No-Core CI calculations of light nuclei: Emergence of rotational bands

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SciDAC project – NUCLEI
lead PI: Joe Carlson (LANL)
http://computingnuclei.org

PetaApps award
lead PI: Jerry Draayer (LSU)

INCITE award – Computational Nuclear Structure
lead PI: James P Vary (ISU)

NERSC

Ab initio nuclear physics – Quantum many-body problem

- Given a Hamiltonian operator

$$\hat{\mathbf{H}} \;=\; \sum_{i<j} \frac{(\vec{p}_i - \vec{p}_j)^2}{2\,m\,A} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

  solve the eigenvalue problem for wavefunction of A nucleons

$$\hat{\mathbf{H}}\,\Psi(r_1,\ldots,r_A) \;=\; \lambda\,\Psi(r_1,\ldots,r_A)$$

  - eigenvalues λ discrete (quantized) energy levels
  - eigenvectors: $|\Psi(r_1,\ldots,r_A)|^2$ probability density for finding nucleons 1, …, A at r_1, …, r_A
- Self-bound quantum many-body problem, with $3(A-1)$ degrees of freedom
- Not only 2-body interactions, but also intrinsic 3-body interactions and possibly 4- and higher N-body interactions
- Strong interactions, with both short-range and long-range pieces

No-Core Configuration Interaction calculations

Barrett, Navrátil, Vary, *Ab initio no-core shell model*, PPNP69, 131 (2013)

- Expand wavefunction in basis states $|\Psi\rangle = \sum a_i |\Phi_i\rangle$
- Express Hamiltonian in basis $\langle\Phi_j|\hat{\mathbf{H}}|\Phi_i\rangle = H_{ij}$
- Diagonalize Hamiltonian matrix H_{ij}
- No-Core Configuration Interaction
  - all A nucleons are treated the same
- Complete basis $\longrightarrow$ exact result
  - caveat: complete basis is infinite dimensional
- In practice
  - truncate basis
  - study behavior of observables as function of truncation
- Computational challenge
  - construct large $(10^{10} \times 10^{10})$ sparse symmetric real matrix H_{ij}
  - use Lanczos algorithm to obtain lowest eigenvalues & -vectors

NCCI – Basis space expansion

- Expand wavefunction in basis $\Psi(r_1, \ldots, r_A) = \sum a_i \Phi_i(r_1, \ldots, r_A)$
- Many-Body basis states $\Phi_i(r_1, \ldots, r_A)$ Slater Determinants of Single-Particle states $\phi_{ik}(r_k)$

$$\Phi_i(r_1, \ldots, r_A) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_{i1}(r_1) & \phi_{i2}(r_1) & \ldots & \phi_{iA}(r_1) \\ \phi_{i1}(r_2) & \phi_{i2}(r_2) & \ldots & \phi_{iA}(r_2) \\ \vdots & \vdots & & \vdots \\ \phi_{i1}(r_A) & \phi_{i2}(r_A) & \ldots & \phi_{iA}(r_A) \end{vmatrix}$$

- Single-Particle basis states $\phi_{ik}(r_k)$
  - eigenstates of SU(2) operators $\hat{\mathbf{L}}^2$, $\hat{\mathbf{S}}^2$, $\hat{\mathbf{J}}^2 = (\hat{\mathbf{L}} + \hat{\mathbf{S}})^2$, and $\hat{\mathbf{J}}_\mathbf{z}$ with quantum numbers n, l, s, j, m
  - radial wavefunctions
    - Harmonic Oscillator
    - Wood–Saxon basis
    - Coulomb–Sturmian
    - ...

Negoita, PhD thesis 2010

Caprio, Maris, Vary, PRC86, 034312 (2012)

NCCI – Truncation schemes

- M-scheme: Many-Body basis states eigenstates of $\hat{\mathbf{J}}_\mathbf{z}$

$$\hat{\mathbf{J}}_\mathbf{z}|\Phi_i\rangle \quad = \quad M|\Phi_i\rangle \quad = \sum_{k=1}^{A} m_{ik}|\Phi_i\rangle$$

  - single run gives entire spectrum
  - alternatives:
    Coupled-J scheme, Symplectic basis, . . .

- N_{max} truncation: Many-Body basis states satisfy

$$\sum_{k=1}^{A} \left(2\, n_{ik} + l_{ik}\right) \;\leq\; N_0 + N_{\text{max}}$$

  - exact factorization of Center-of-Mass motion

- Alternatives:
  - Importance Truncation — Roth, PRC79, 064324 (2009)
  - No-Core Monte-Carlo Shell Model — Abe *et al*, PRC86, 054301 (2012)
  - SU(3) Truncation — Dytrych *et al*, PRL111, 252501 (2013)
  - . . .

Intermezzo: Center-of-Mass excitations

- Use single-particle coordinates, not relative (Jacobi) coordinates
  - straightforward to extend to many particles
  - have to separate Center-of-Mass motion from relative motion
- Center-of-Mass wavefunction factorizes for H.O. basis functions in combination with $N_{\max}$ truncation

$$\begin{aligned} |\Psi_{\text{total}}\rangle &= |\phi_1\rangle \otimes \ldots \otimes |\phi_A\rangle \\ &= |\Phi_{\text{Center-of-Mass}}\rangle \otimes |\Psi_{\text{rel}}\rangle \end{aligned}$$

where

$$\hat{\mathbf{H}}_{\text{rel}} |\Psi_{\text{j, rel}}\rangle = E_{\text{j}} |\Psi_{\text{j, rel}}\rangle$$

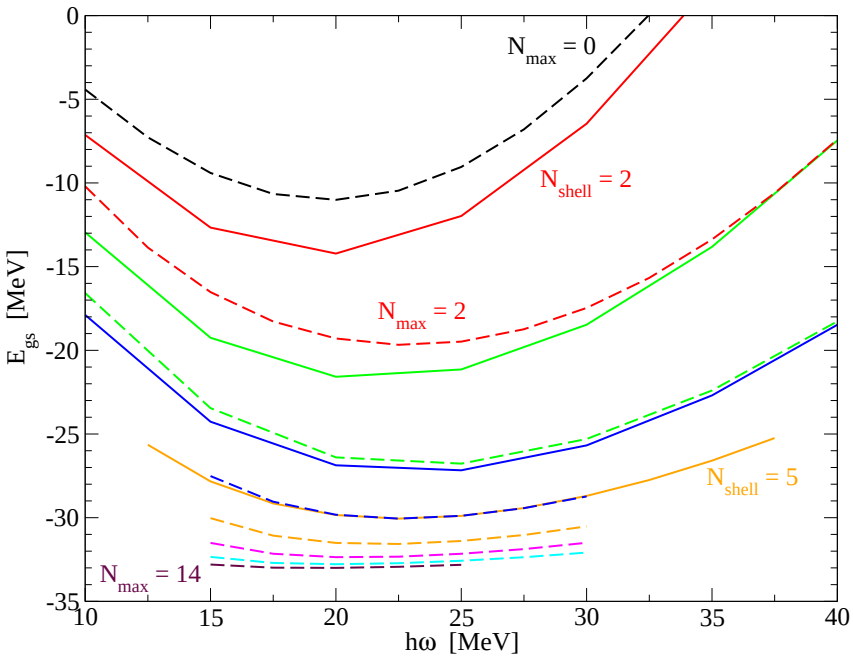
- Add Lagrange multiplier to Hamiltonian (Lawson term)

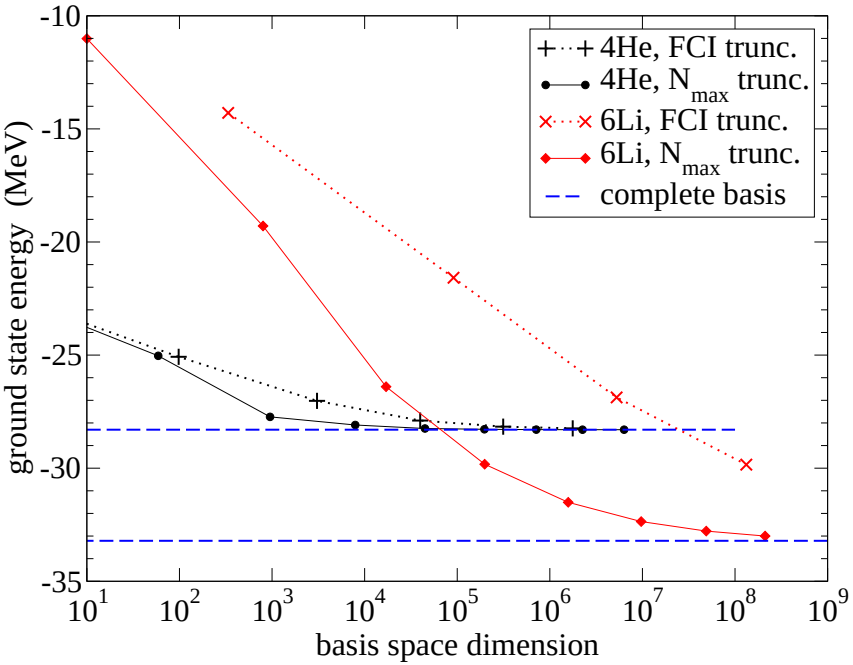
$$\hat{\mathbf{H}}_{\text{rel}} \longrightarrow \hat{\mathbf{H}}_{\text{rel}} + \Lambda_{CM} \left(\hat{\mathbf{H}}^{H.O.}_{CM} - \frac{3}{2}\hbar\omega \right)$$

with $\hat{\mathbf{H}}_{\text{rel}} = \hat{\mathbf{T}}_{\text{rel}} + \hat{\mathbf{V}}_{\text{rel}}$ the relative Hamiltonian

- separates CM excitations from CM ground state $|\Phi_{CM}\rangle$

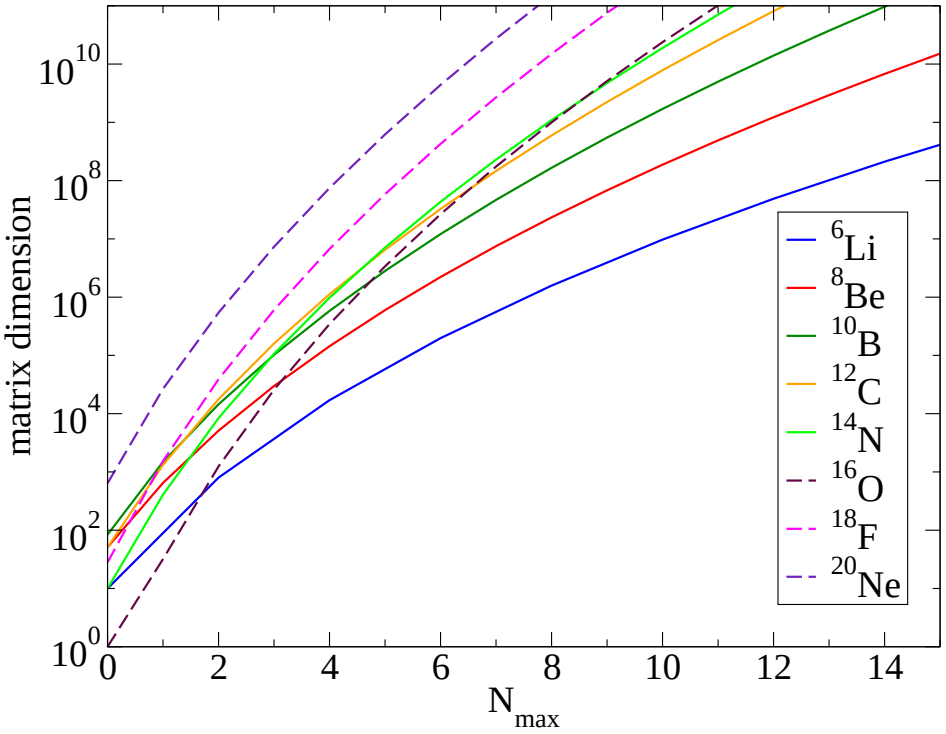
Intermezzo: FCI vs. Nmax truncation

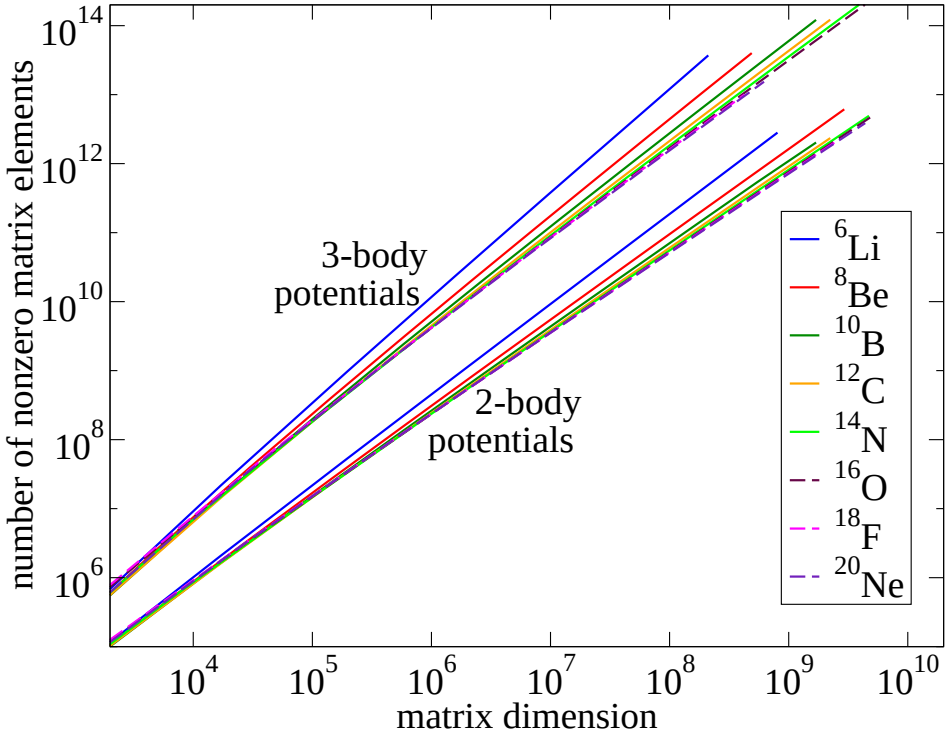




- $N_{\max}$ truncation
  - exact factorization of Center-of-Mass motion
- Infinite basis space limit: No-Core Full Configuration (NCFC)
  - both $N_{\max}$ truncation and FCI converge to the same results
  - $N_{\max}$ truncation does so much more rapidly

NCCI calculations – main challenge





- Increase of basis space dimension with increasing A and N_{max}
  - need calculations up to at least $N_{\text{max}} = 8$
    for meaningful extrapolation and numerical error estimates
- More relevant measure for computational needs
  - number of nonzero matrix elements
  - current limit 10^{13} to 10^{14} (Edison, Mira, Titan)

Many Fermion Dynamics – nuclear physics

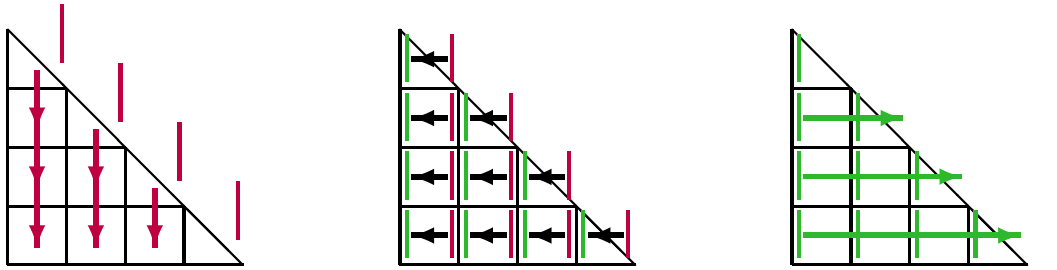
Configuration Interaction code for nuclear structure calculations

- Platform-independent, hybrid OpenMP/MPI, Fortran 90
- Generate many-body basis space
  subject to user-defined single-particle and many-body truncation
- Construct of many-body matrix H_{ij}
  - determine which matrix elements can be nonzero
    based on quantum numbers of underlying single-particle states
  - evaluate and store nonzero matrix elements
    in compressed row/column format
- Obtain lowest eigenpairs using Lanczos algorithm
  - typical use: 10 to 20 lowest eigenvalues and eigenvectors
  - typically need $\sim$ 400 to $\sim$ 800 Lanczos iterations
  - some applications need hundreds of eigenvalues
- Write eigenvectors (wavefunctions) to disk
- Calculate selected set of observables

MFDn – 2-dimensional distribution of matrix

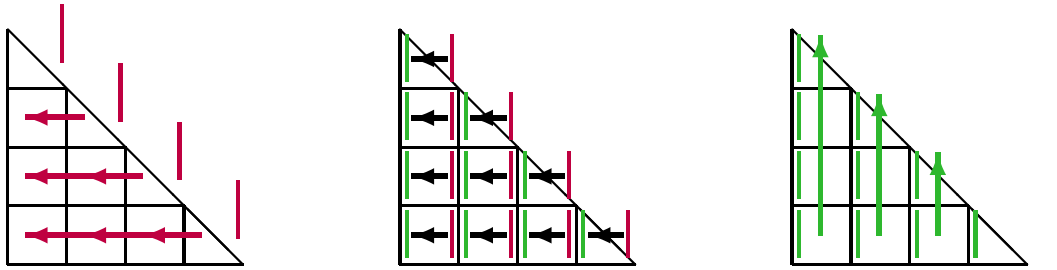
- Real symmetric matrix: store only lower (or upper) triangle distributed over $n = d \cdot (d+1)/2$ processors with d "diagonal" proc's
- In principle, we can deal with arbitrary large dimensions even if we cannot store an entire vector on a single processor
- Communication pattern matrix-vector multiplication

lower triangle



BCast(x) $y \leftarrow Ax$ Reduce(y)

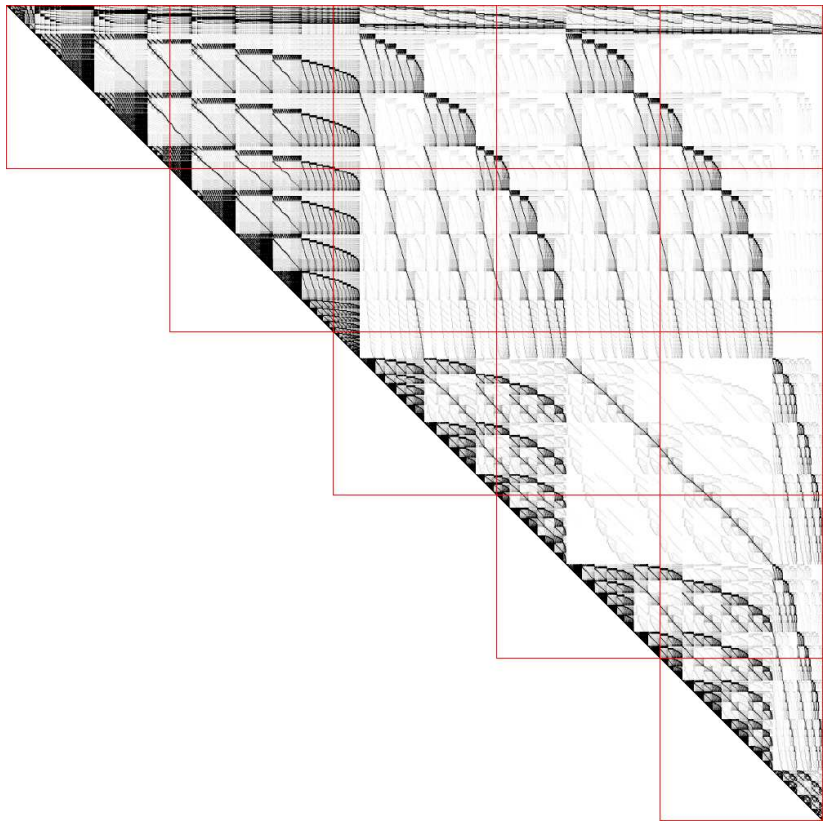
upper triangle

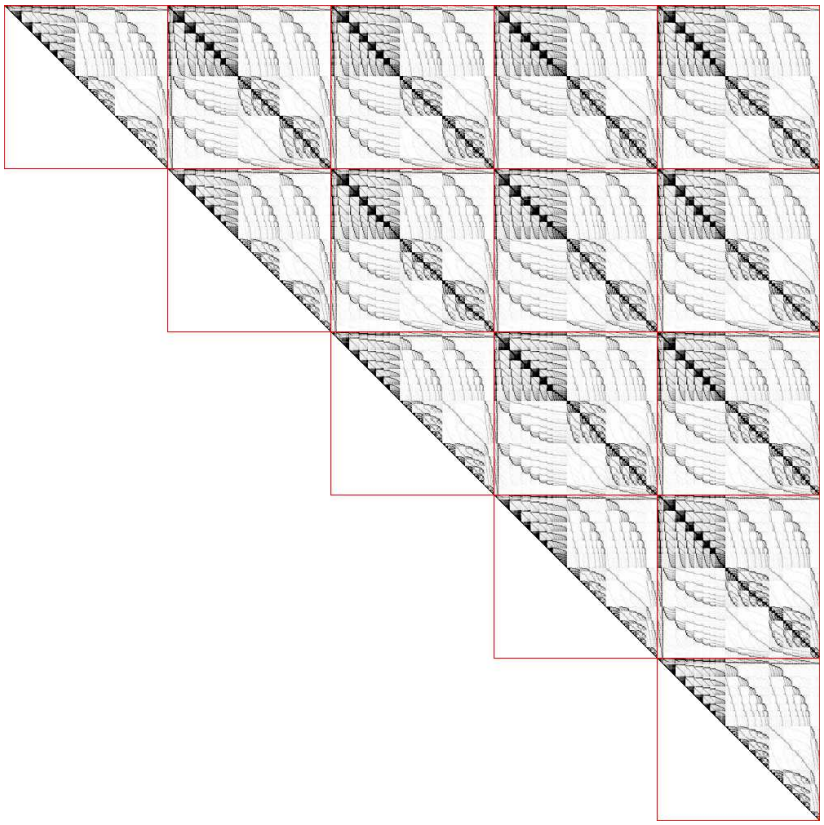


BCast(x) $y \leftarrow A^T x$ Reduce(y)

Load balancing

Round-robin distribution of (groups of) many-body basis states





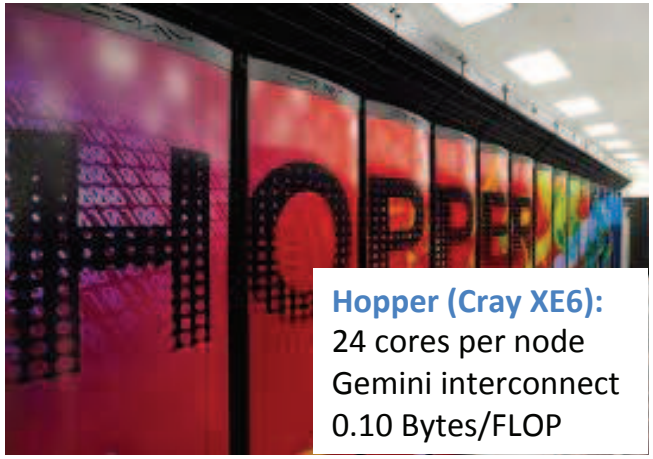
- ^{8}Be at $N_{\max} = 4$ with 3NF on 15 MPI processors
- Dimension 143,792, # nonzero matrix elements 402,513,272

Performance issue with the newer Cray machine

Franklin (Cray XT4):
4 cores per node
Seastar interconnect
1.36 Bytes/FLOP

Same compilers/libraries
for building executables

Identical jobs
^{9}Be(4 protons,5 neutrons)
D= 575 million
nonzeros= 668 billion



Hopper (Cray XE6):
24 cores per node
Gemini interconnect
0.10 Bytes/FLOP

More (and faster) cores on Hopper

Franklin: 2556 nodes, 2556 MPI processors, 4 threads/processor = **10,224 cores**
Hopper: 639 nodes, 2556 MPI processors, 6 threads/processor = **15,336 cores**

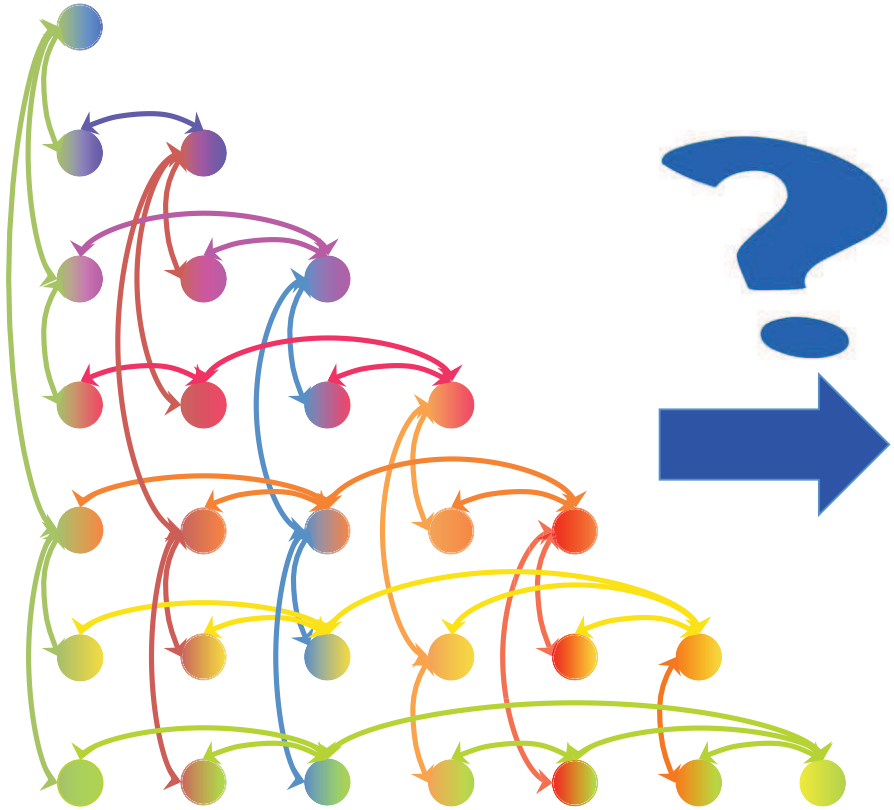
Consumed more resources on Hopper!
39,110 CPU-hours on Franklin
75,325 CPU-hours on Hopper???

Actually took longer to run on Hopper!
3.83 hours on Franklin
4.91 hours on Hopper???

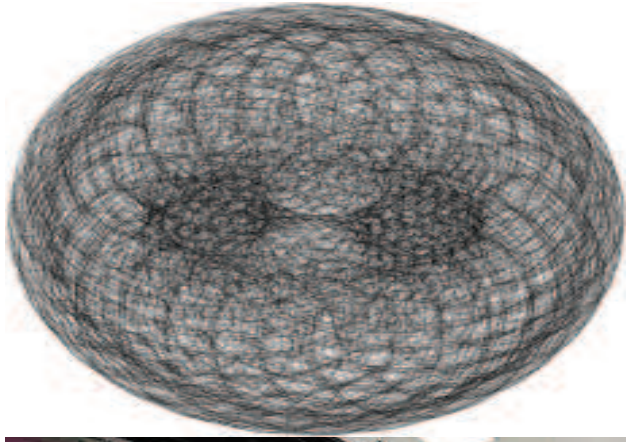
Slide courtesy of Metin Aktulga, LBNL, 2012 (now at MSU)

Topology-aware Mapping

MFDn's communication graph



Hopper's 3D Torus



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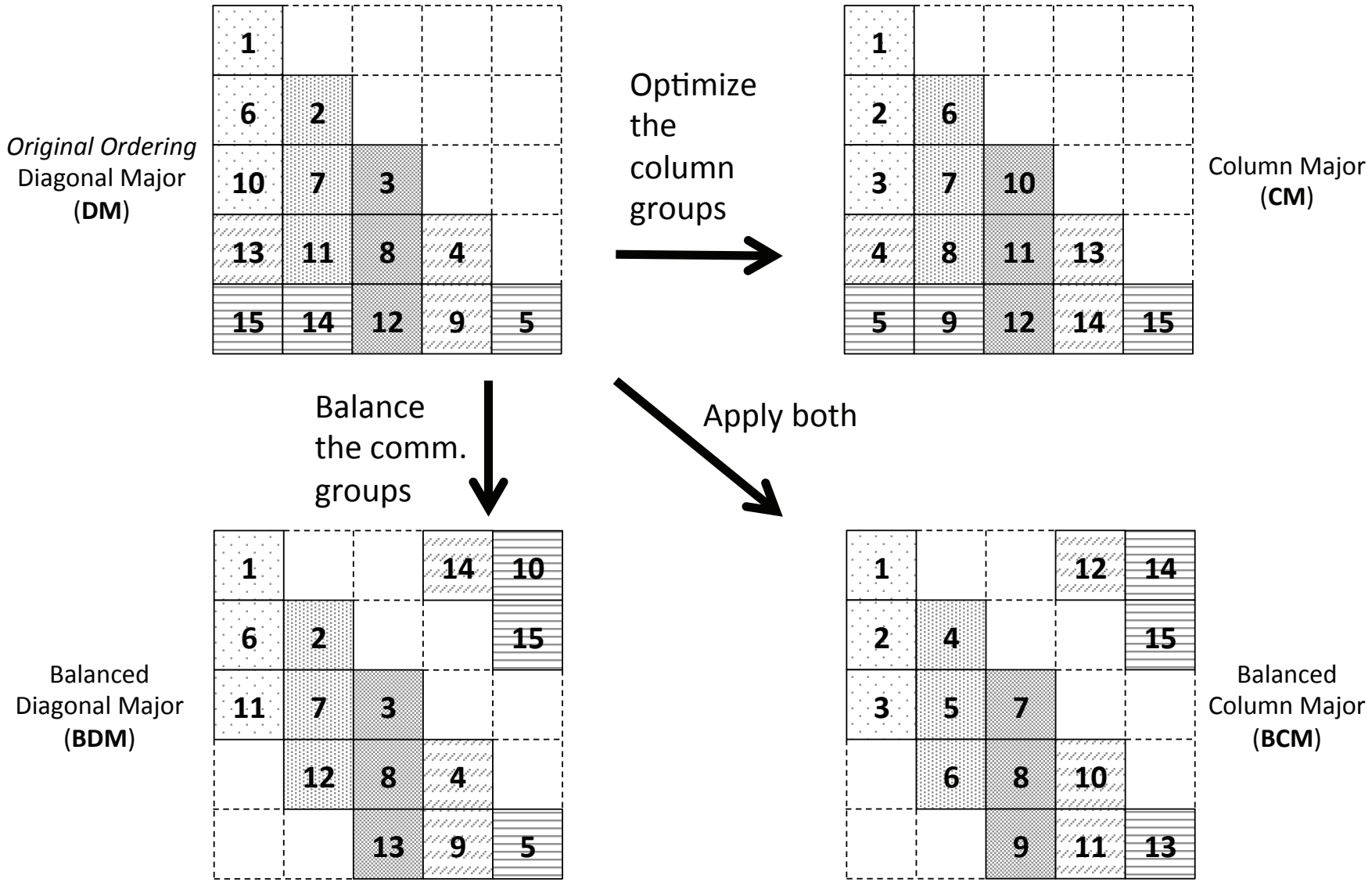
Different Orderings



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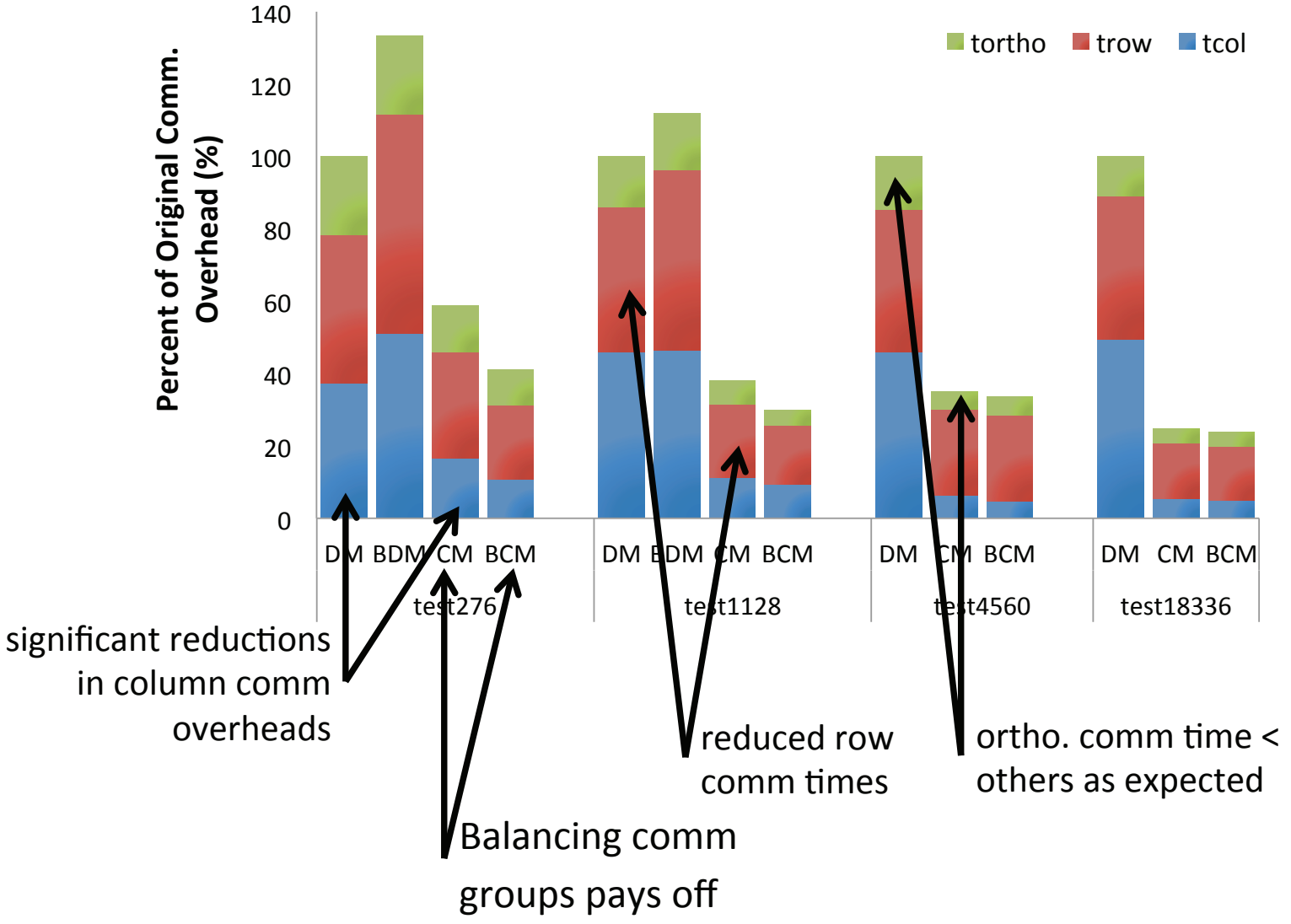
Communication Improvement



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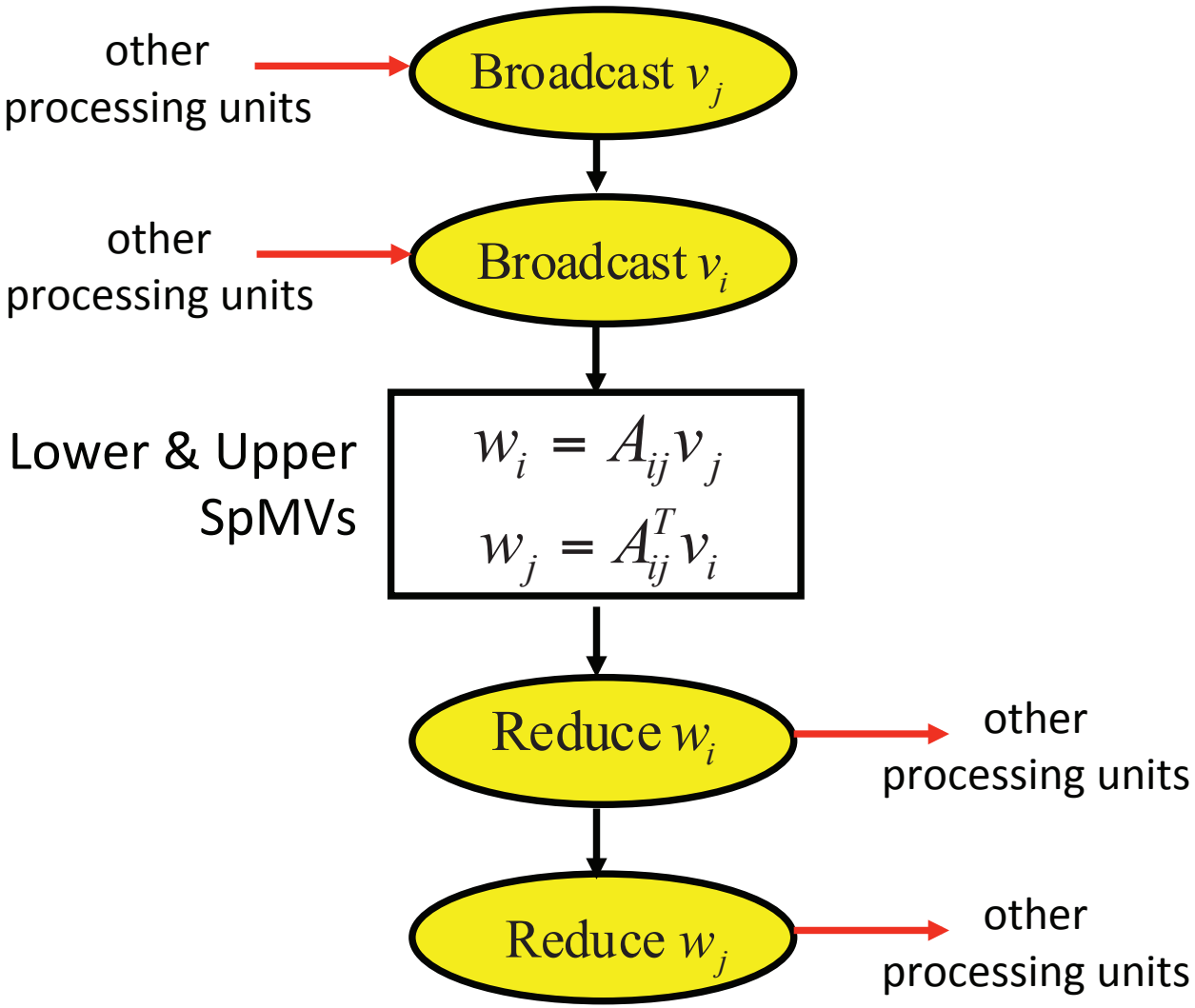
Communication Hiding: Main Idea



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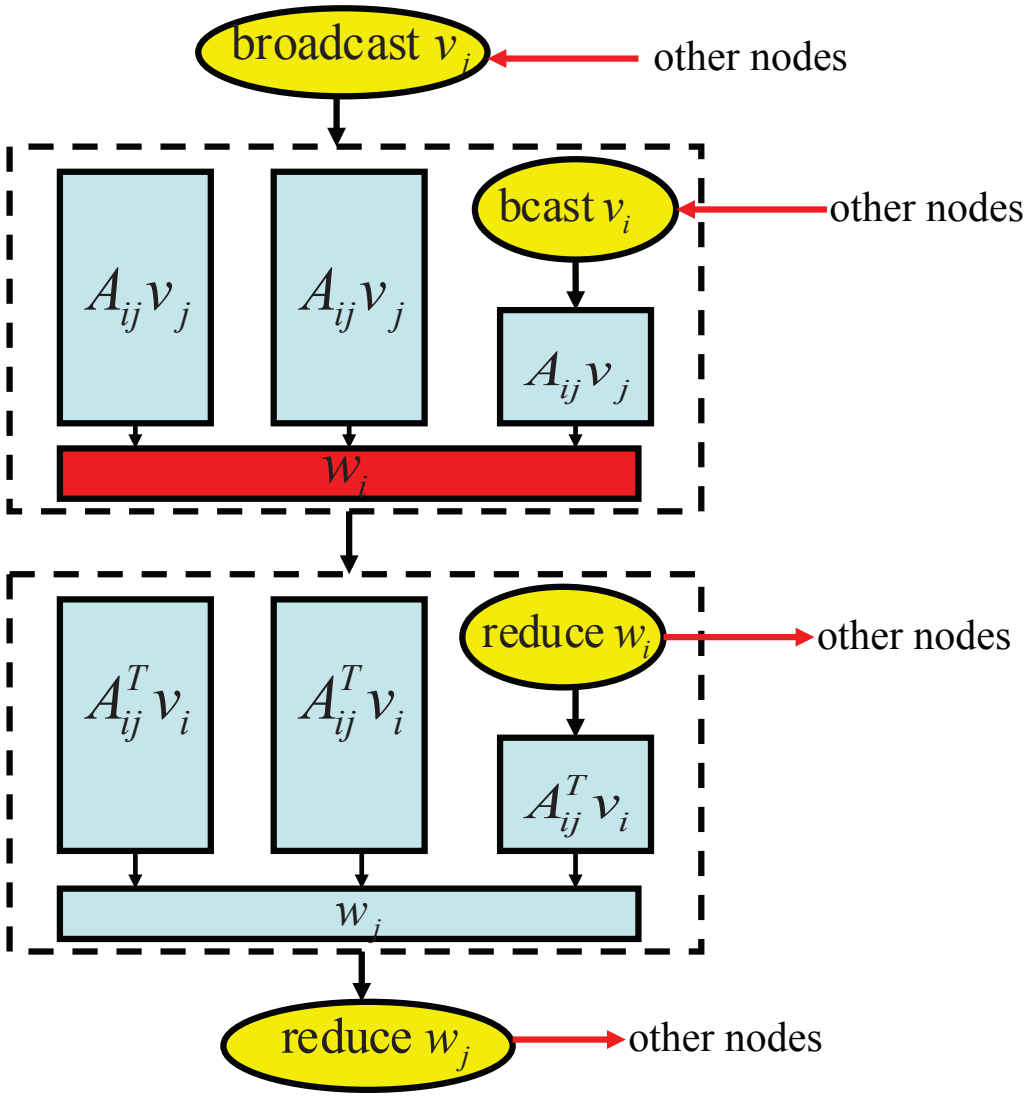
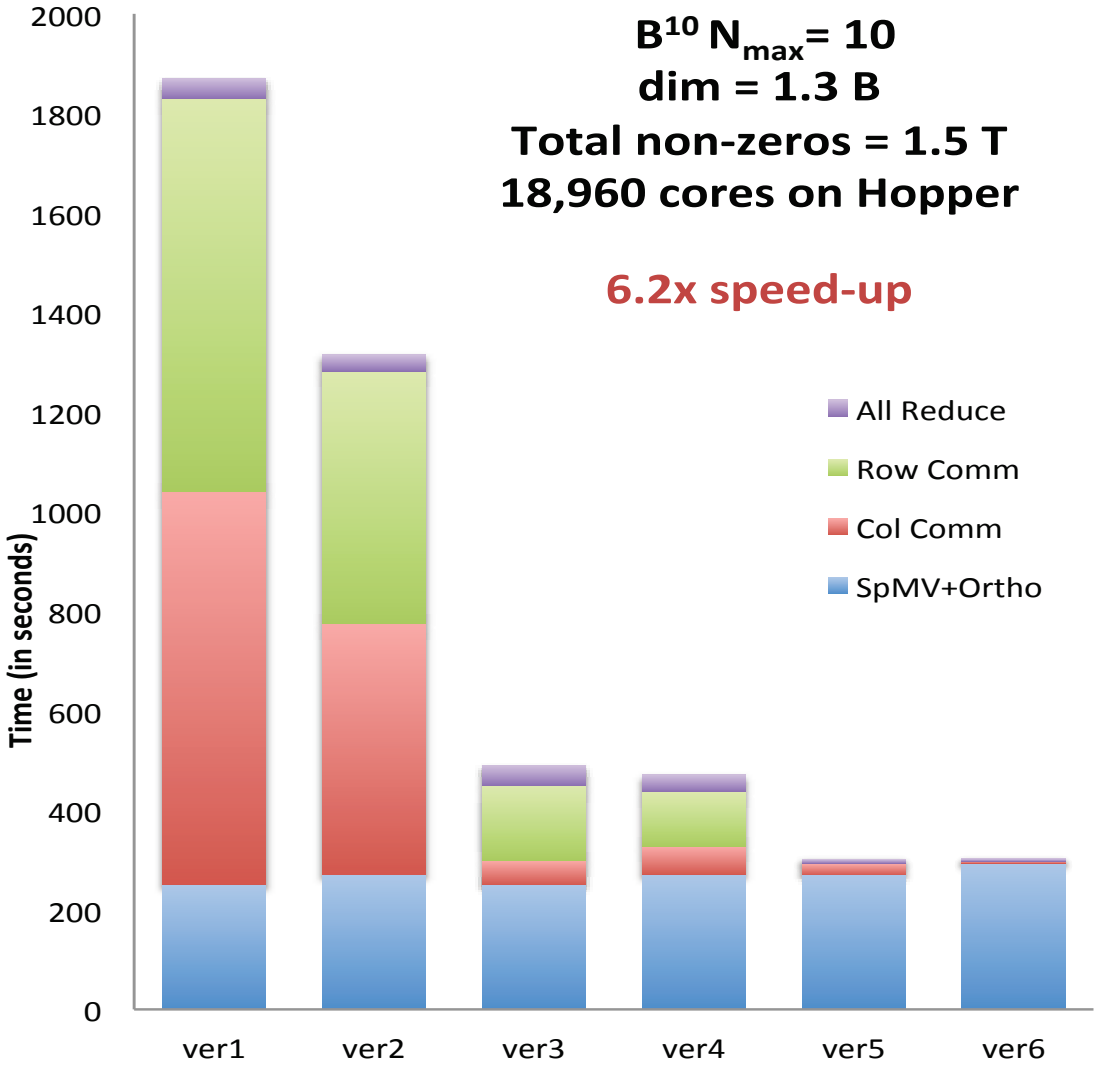


Slide courtesy of Metin Aktulga, LBNL, 2012 (now at MSU)

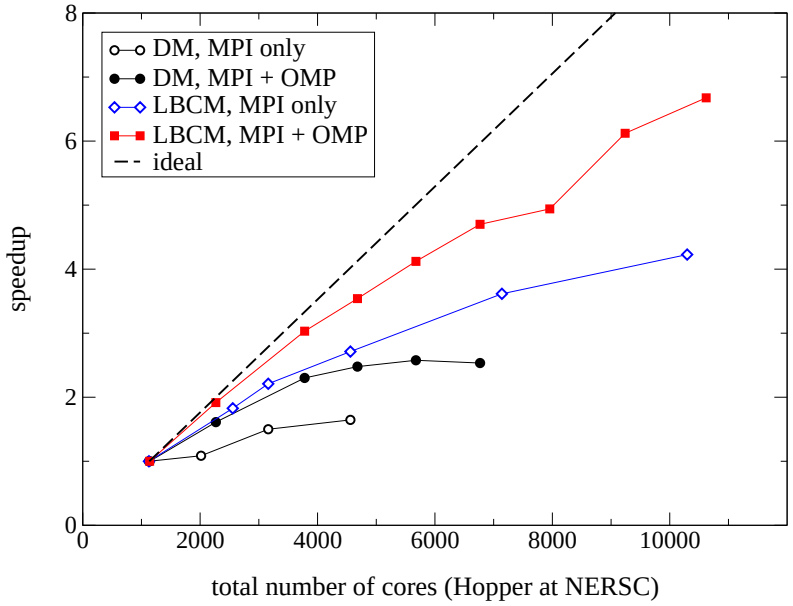
Performance Results

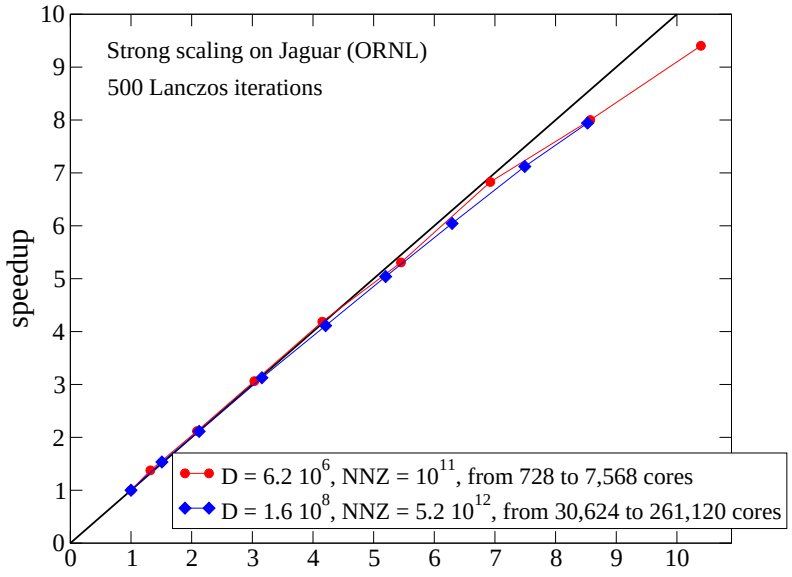


Slide courtesy of Metin Aktulga, LBNL, 2012 (now at MSU)

Strong Scaling of MFDn

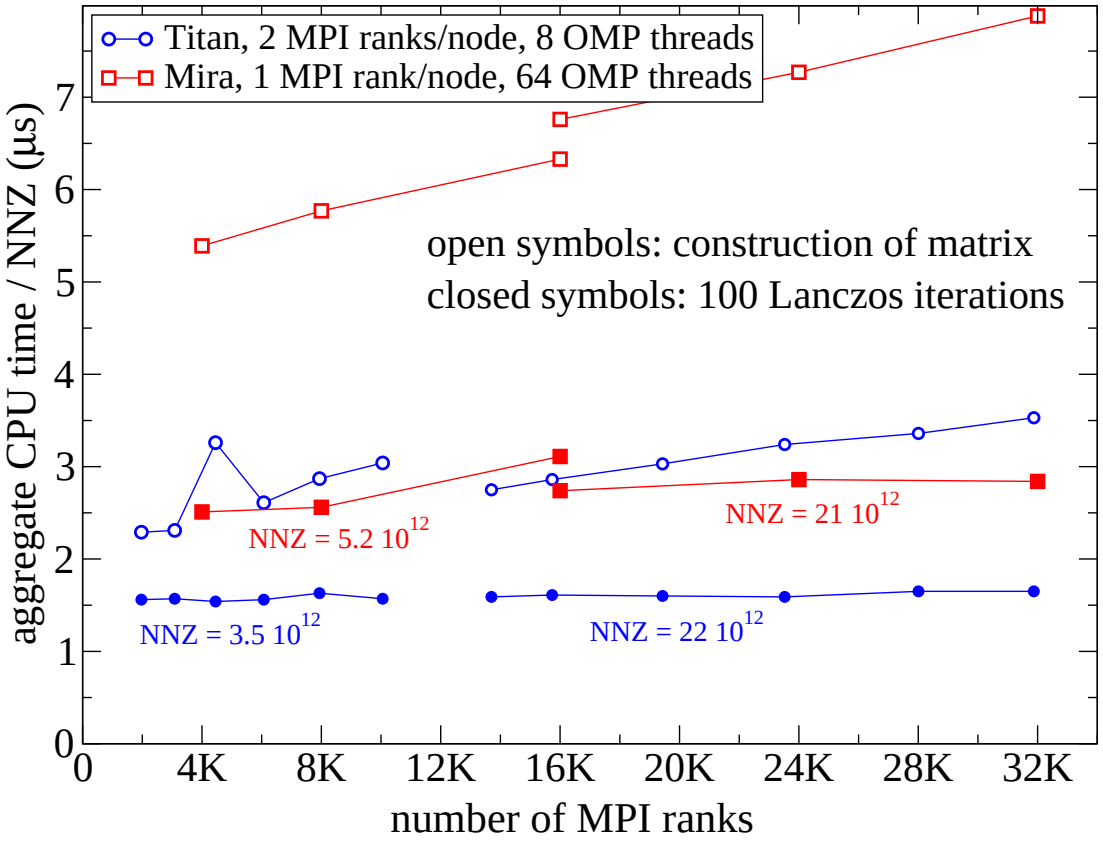
Aktulga, Yang, Ng, Maris, Vary, Concurrency Computat.: Pract. Exper. (2013)





- Understand communication overheads in terms of heuristic network model based on set of compute nodes, physical links between compute nodes, and link capacity
- Hybrid OpenMP/MPI with 1 MPI processor per NUMA node performs better than MPI-only for more than few hundred cores
- Runs with 3-body forces scale better than NN-only runs

Scaling of MFDn on Leadership Class Facilities



- Version14 Beta03, June 2013
- 2-body + 3-body forces
- 100 Lanczos iterations

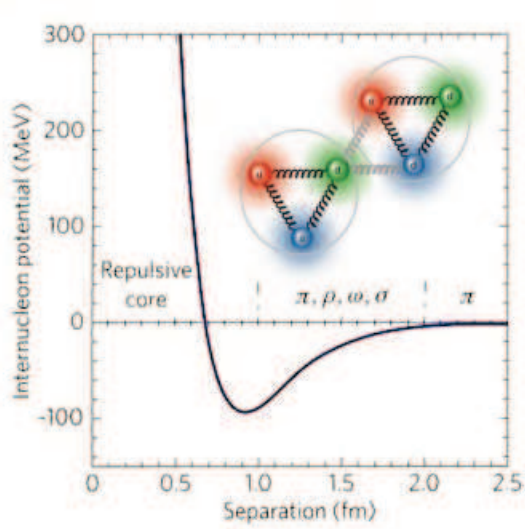
- Titan: Cray XK7 with 2.2 GHz AMD Opteron 16-core CPU with 32 GB per node (plus NVIDIA Kepler GPUs)
- Mira: IBM BG/Q with 1.6 GHz 16-core CPU with 16 GB per node (supporting up to 64 threads)

Nuclear interaction

Nuclear potential not well-known,

though in principle calculable from QCD

$$\hat{\mathbf{H}} = \hat{\mathbf{T}}_{\text{rel}} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$



In practice, alphabet of realistic potentials

- Argonne potentials: AV8′, AV18
  - plus Urbana 3NF (UIX)
  - plus Illinois 3NF (IL7)
- Bonn potentials
- Chiral NN interactions
  - plus chiral 3NF, ideally to the same order
- ...
- JISP16
- ...

Phenomeological NN interaction: JISP16

JISP16 tuned up to ^{16}O

- Constructed to reproduce np scattering data
- Finite rank seperable potential in H.O. representation
- Nonlocal NN-only potential
- Use Phase-Equivalent Transformations (PET) to tune off-shell interaction to
  - binding energy of ^{3}H and ^{4}He
  - low-lying states of ^{6}Li (JISP6, precursor to JISP16)
  - binding energy of ^{16}O

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Realistic nuclear Hamiltonian: Ab exitu approach

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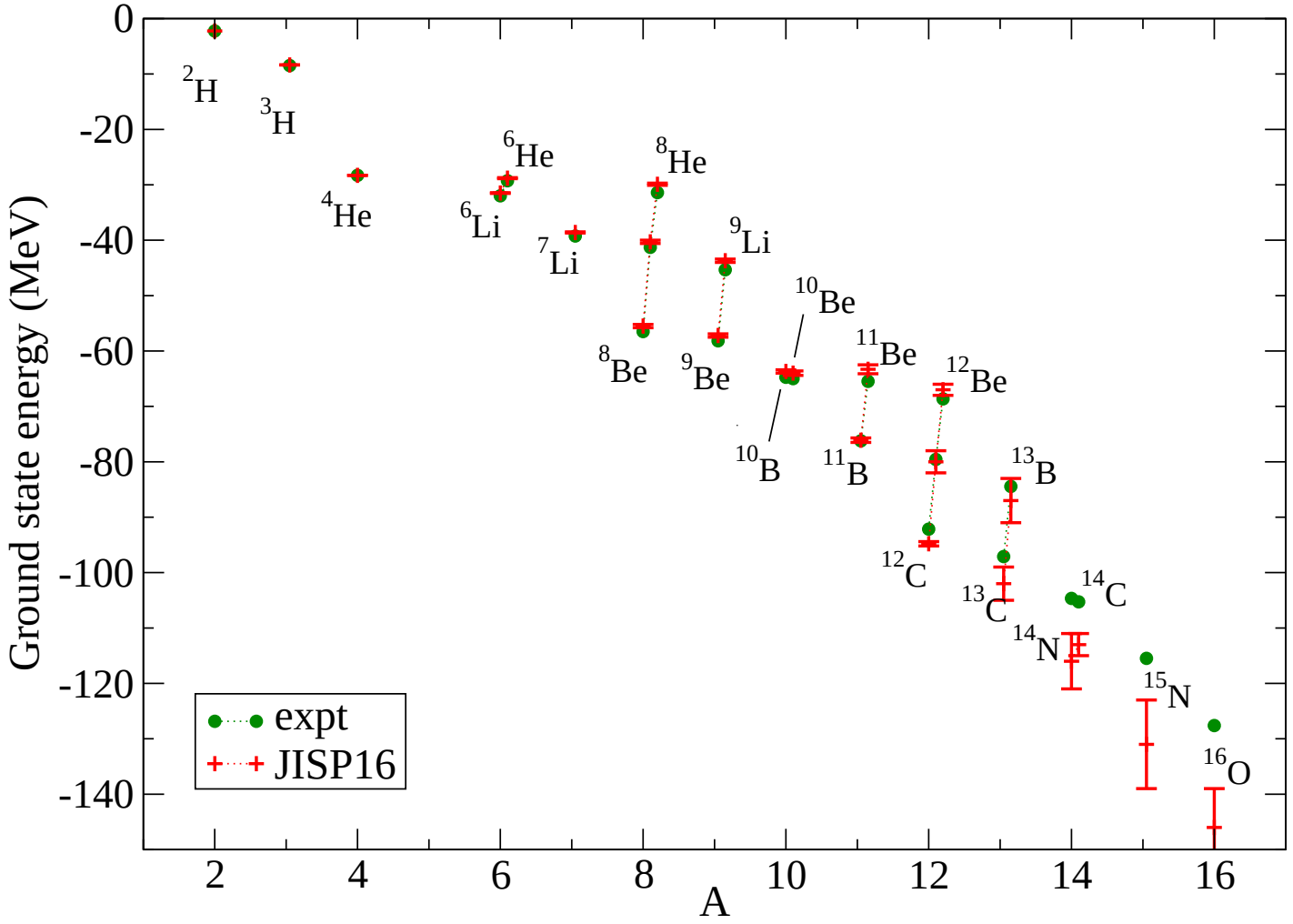
Ground state energy of p-shell nuclei with JISP16

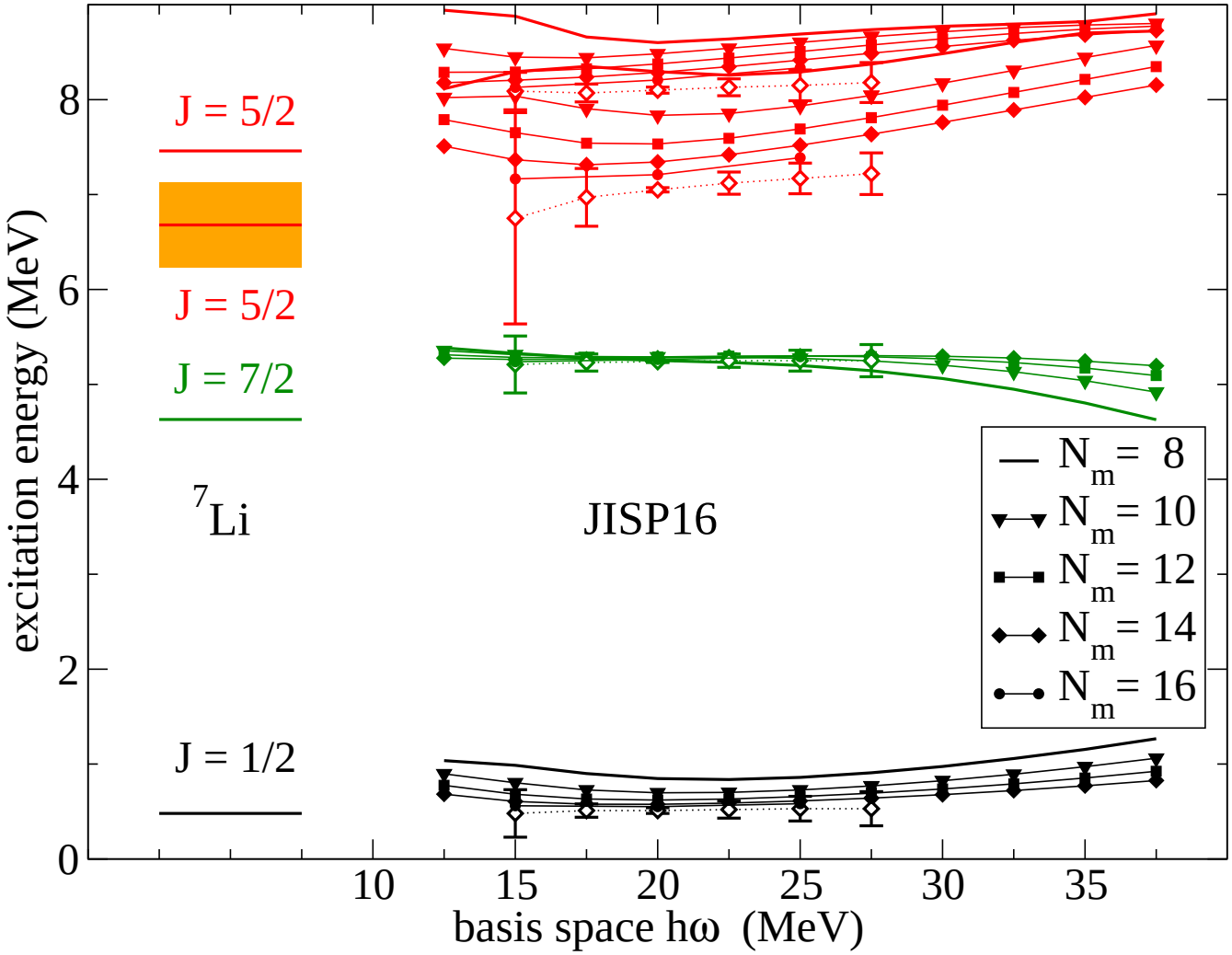
Maris, Vary, IJMPE22, 1330016 (2013)



- ^{10}B – most likely JISP16 produces correct 3^+ ground state, but extrapolation of 1^+ states not reliable due to mixing of two 1^+ states
- ^{11}Be – expt. observed parity inversion within error estimates of extrapolation
- ^{12}B and ^{12}N – unclear whether gs is 1^+ or 2^+ (expt. at $E_x = 1$ MeV) with JISP16

Excitation spectrum 7Li

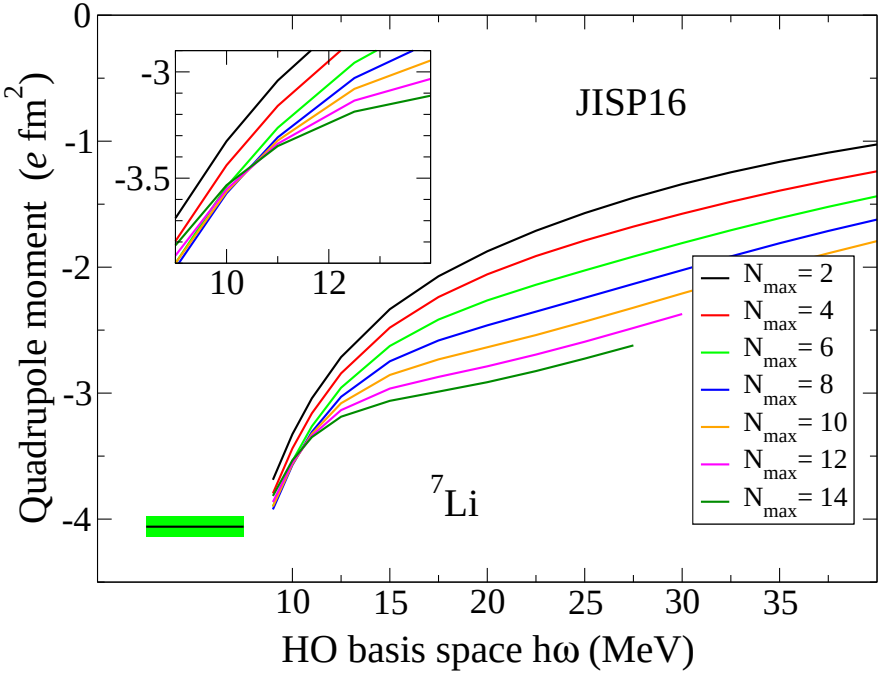
Cockrell, Maris, Vary, PRC86 034325 (2012)

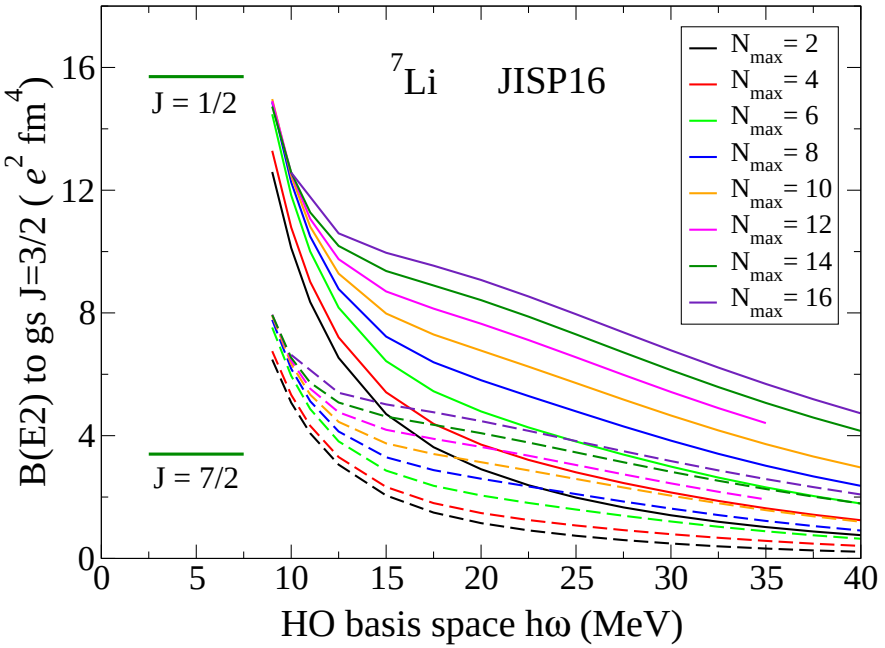


- Narrow states well converged, no extrapolation needed
- Broad resonances generally not as well converged; may need to incorporate continuum?

Quadrupole moment and B(E2) transition strengths 7Li

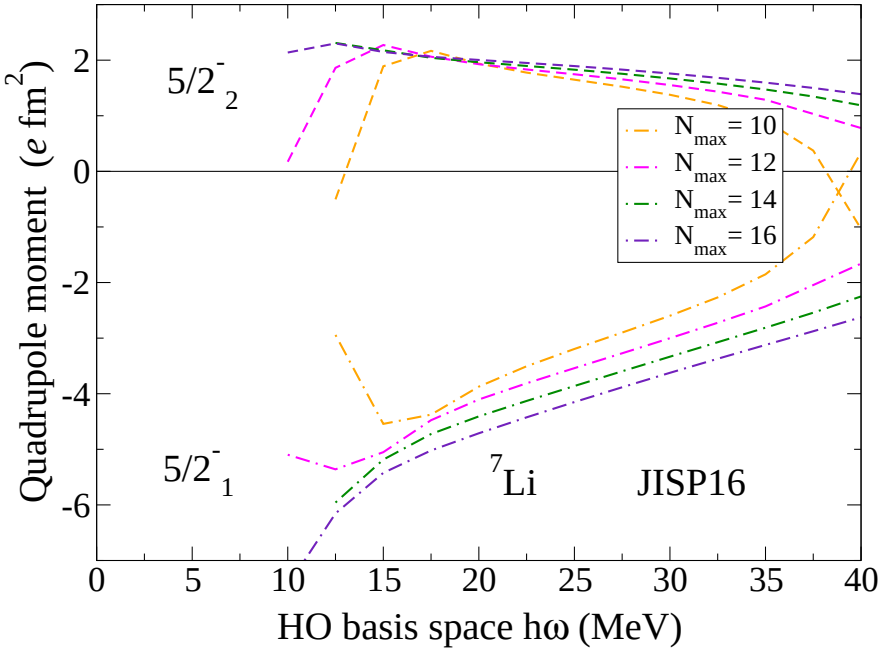
Cockrell, Maris, Vary, PRC86 034325 (2012)

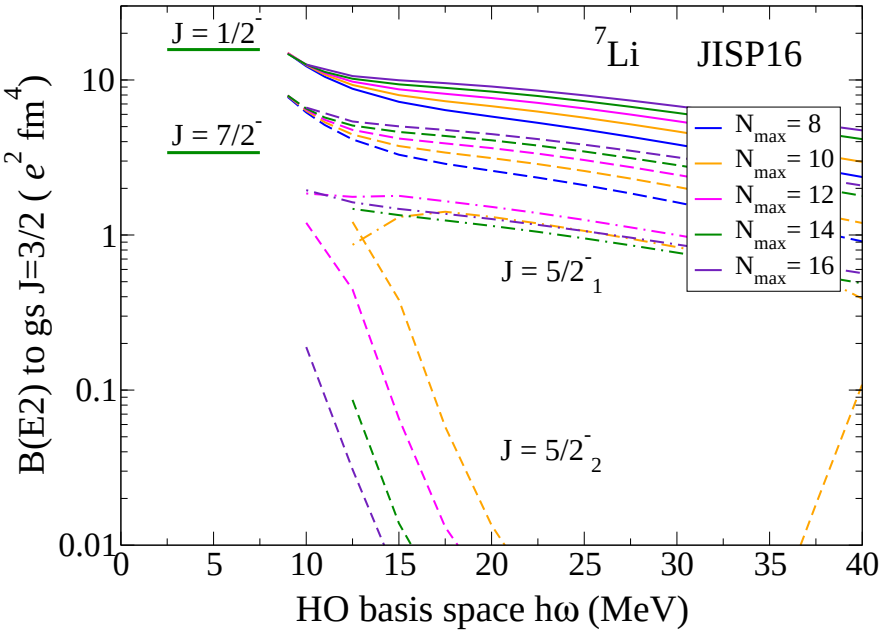




- E2 observables not converged,
  due to gaussian fall-off of HO wavefunction
- Nevertheless, qualitative agreement of Q and B(E2) with data

Quadrupole moments and B(E2) transitions for $J^\pi = \frac{5}{2}^-$ states

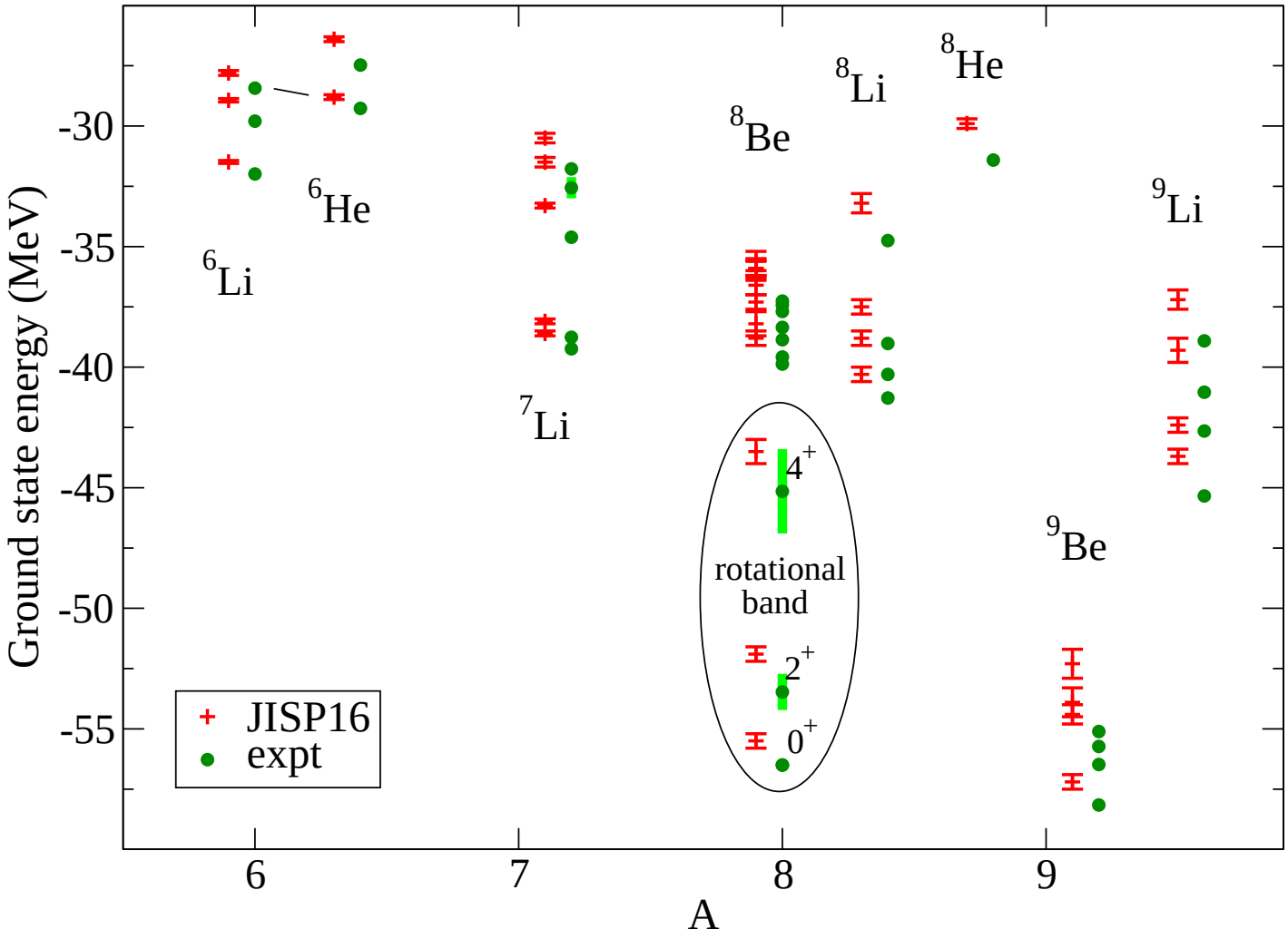




- E2 observables not converged, but nevertheless
  - $J^\pi = \left(\frac{5}{2}^-\right)_1$ large negative quadrupole moment
  - $\frac{1}{2}^-$, $\frac{7}{2}^-$, and $\left(\frac{5}{2}^-\right)_1$ relatively strong B(E2) to g.s.
  - $J^\pi = \left(\frac{5}{2}^-\right)_2$ small positive quadrupole moment, $Q \sim 2\ e$ fm^2, and very small B(E2) to g.s.

Energies of narrow A=6 to A=9 states with JISP16

Maris, Vary, IJMPE22, 1330016 (2013)



- Excitation spectrum narrow states in good agreement with data

Intermezzo: Rotational states

Assuming adiabatic separation of rotational and internal degrees of freedom, a rotational nuclear state $|\psi_{JKM}\rangle$ can be described in terms of an intrinsic state $|\phi_K\rangle$ in a non-inertial frame, combined with the rotational motion of this non-inertial frame

$$|\psi_{JKM}\rangle \quad = \quad \mathcal{N}_{JK} \int d\vartheta \left[\mathscr{D}^J_{MK}(\vartheta)|\phi_K;\vartheta\rangle + (-)^{J+K}\mathscr{D}^J_{M-K}(\vartheta)|\phi_{\bar{K}};\vartheta\rangle\right]$$

- Rotational energy

$$E(J) \quad = \quad E_0 + \frac{\hbar^2}{2\mathcal{I}}\ (J(J+1))$$

for $K = \frac{1}{2}$ bands staggering due to Coriolis term

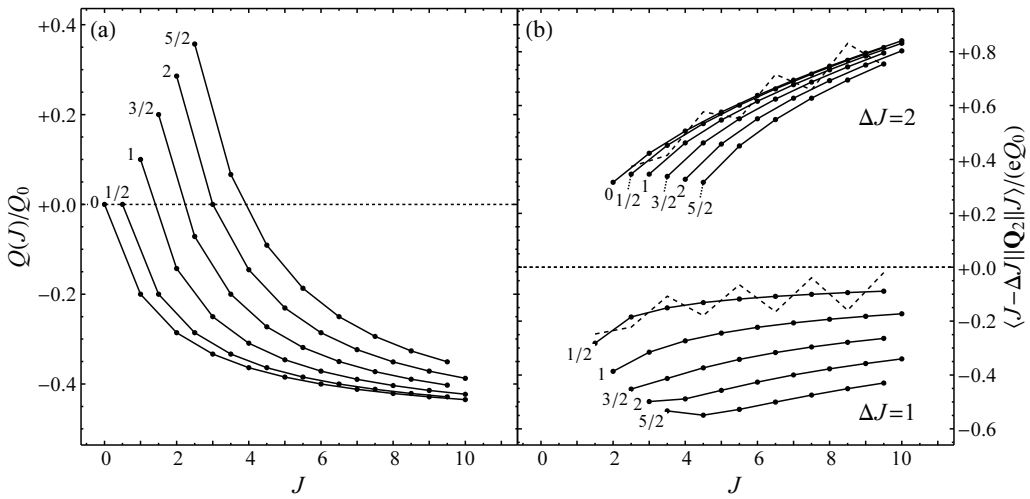
$$E(J) \quad = \quad E_0 + \frac{\hbar^2}{2\mathcal{I}}\ \left(J(J+1) + a\,(-1)^{J+\frac{1}{2}}\ (J+\tfrac{1}{2})\right)$$

Rotational states: Quadrupole matrix elements

$$\langle \psi_{J_f K} || E_2 || \psi_{J_i K} \rangle = \frac{(2J_i+1)^{1/2}}{1+\delta_{K0}} \Big((J_i, K, 2, 0 | J_f, K) \, \langle \phi_K || E_{2,0} || \phi_K \rangle + (-)^{J_i+K} (J_i, -K, 2, 2K | J_f, K) \, \langle \phi_K || E_{2,2K} || \phi_{\bar{K}} \rangle \Big)$$

- Consider both proton and neutron quadrupole tensors
- Quadrupole moments

$$\mathcal{Q}(J) = \frac{3K^2 - J(J+1)}{(J+1)(2J+3)} \, \mathcal{Q}_0$$



- Transition matrix elements

$$\langle \psi_{J_f K} || E_2 || \psi_{J_i K} \rangle = \sqrt{\frac{5}{16\pi}} \, \sqrt{2J_i+1} \, (J_i K 20 | J_f K) \, \mathcal{Q}_0$$

Rotational states: Dipole matrix elements

- Magnetic moments

$$\mu(J) \quad = \quad a_0\, J + a_1\, \frac{K}{J+1} + a_2\, \delta_{K,\frac{1}{2}}\, \frac{(-1)^{J-\frac{1}{2}}}{2\sqrt{2}}\, \frac{2J+1}{J+1}$$

- Magnetic transition matrix elements

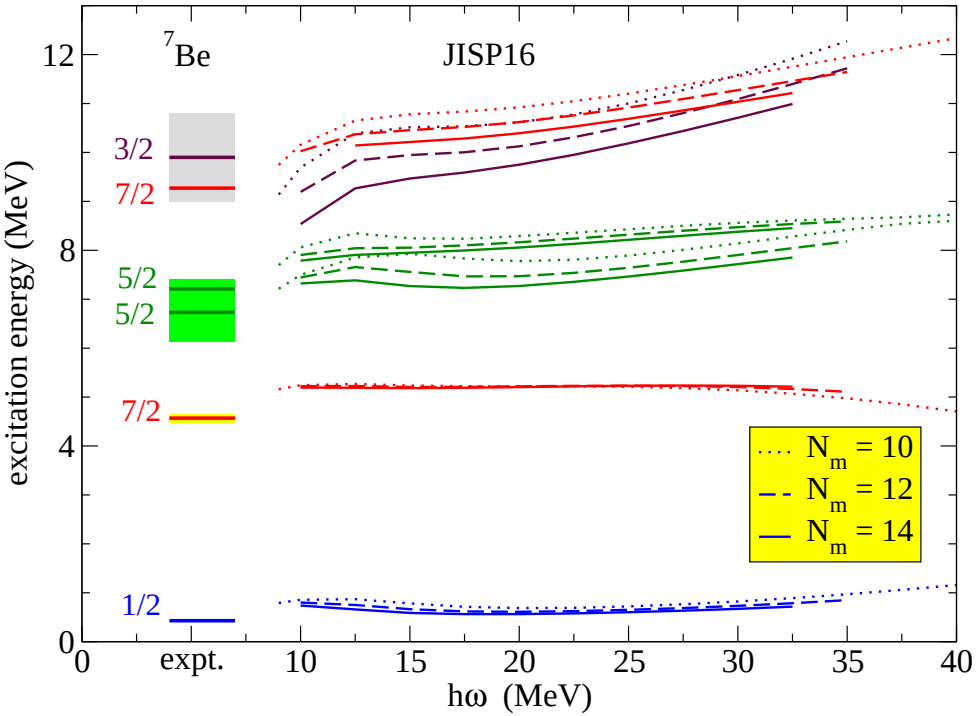
$$\langle \psi_{J-1,K} || M_1 || \psi_{J,K} \rangle \quad = \quad -\sqrt{\frac{3}{4\pi}}\, \sqrt{\frac{J^2-K^2}{J}}\, \left(a_1 + a_2\, \delta_{K,\frac{1}{2}}\, \frac{(-1)^{J-\frac{1}{2}}}{\sqrt{2}} \right)$$

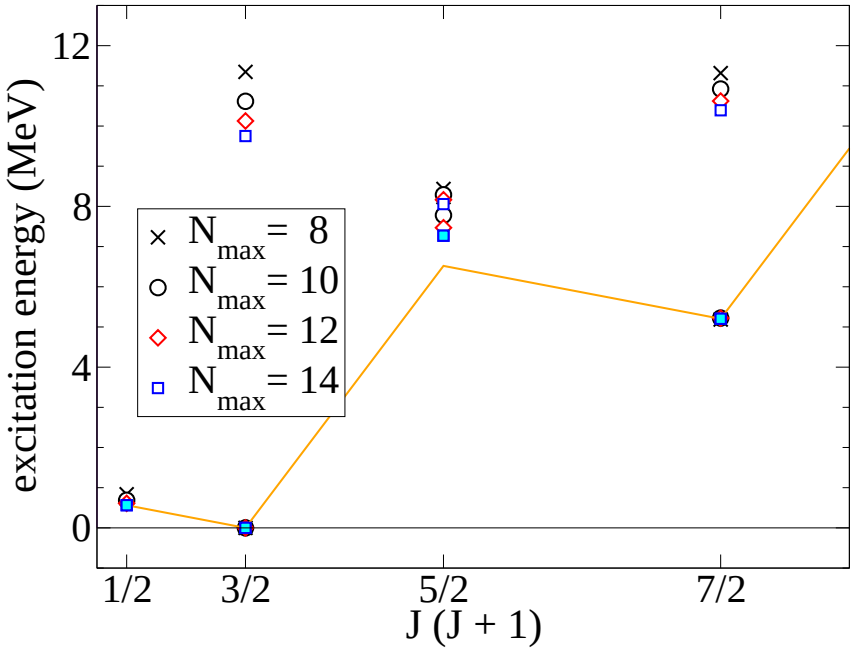
- Define dipole terms $D_{l,p}$, $D_{l,n}$, $D_{s,p}$, and $D_{s,n}$ for both the magnetic moments and for the M_1 transitions

$$M_1 \quad = \quad g_{l,p}\, D_{l,p} + g_{l,n}\, D_{l,n} + g_{s,p}\, D_{s,p} + g_{s,n}\, D_{s,n}$$

with $g_{l,p} = 1$, $g_{l,n} = 0$, $g_{s,p} = 5.586$, and $g_{s,n} = -3.826$

Excitation spectrum 7Be – Emergence of rotational band?

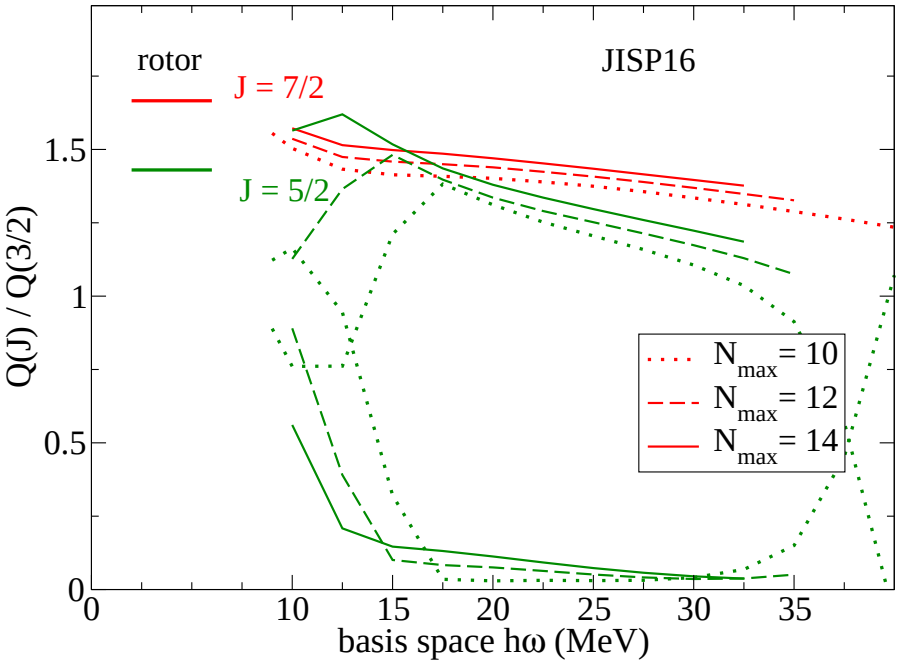


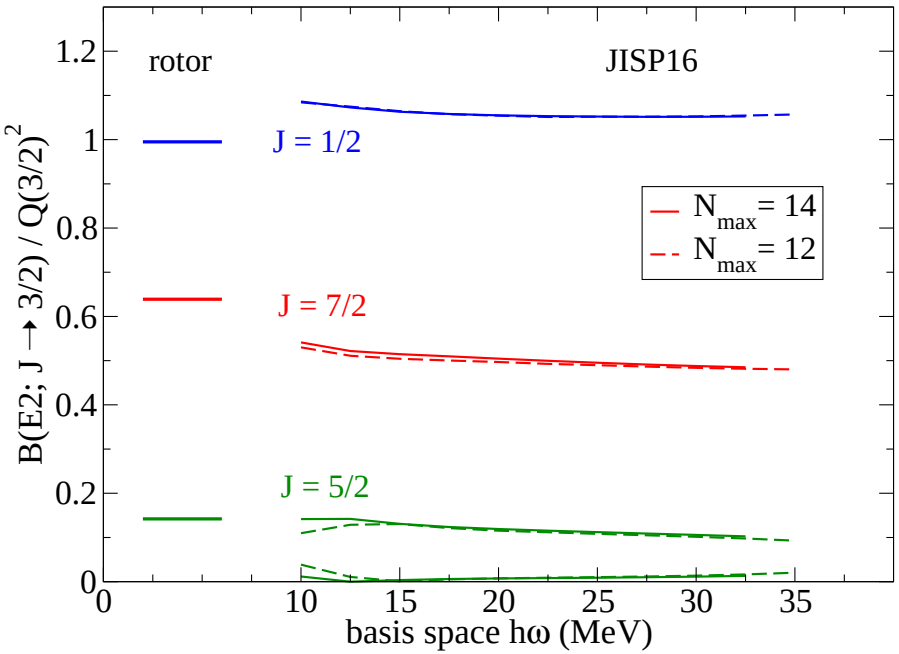


- Spectrum in reasonable agreement with data
  - lowest two excited states converged
  - broad resonances not as well converged
- Excitation energies of lowest J states consistent with $K = \frac{1}{2}$ rotational band

Emergence of $K = \frac{1}{2}$ rotational band

Ratio of electric quadrupole moments and B(E2)'s over ground state quadrupole moment $\mathcal{Q}(3/2)$



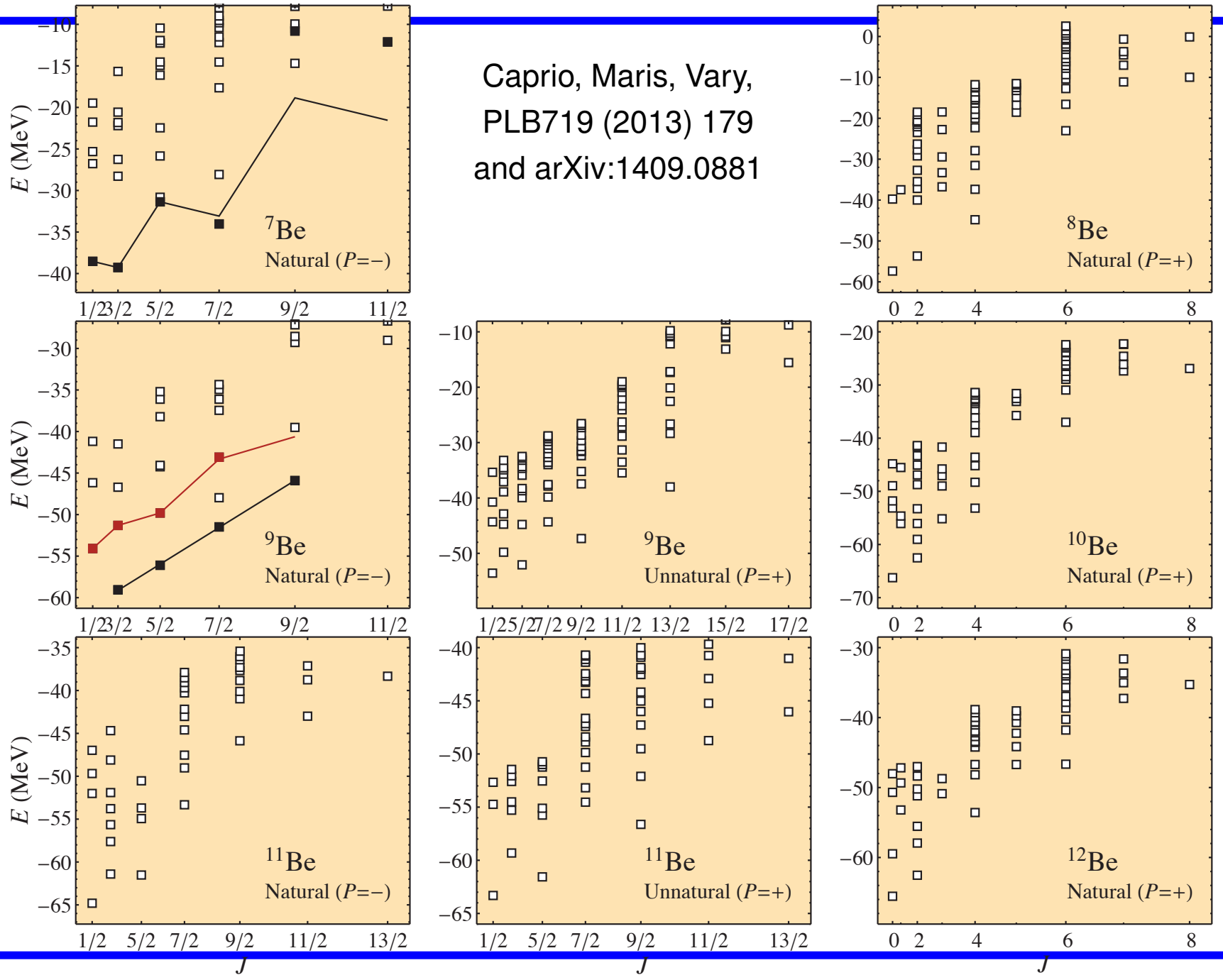


Rotor model

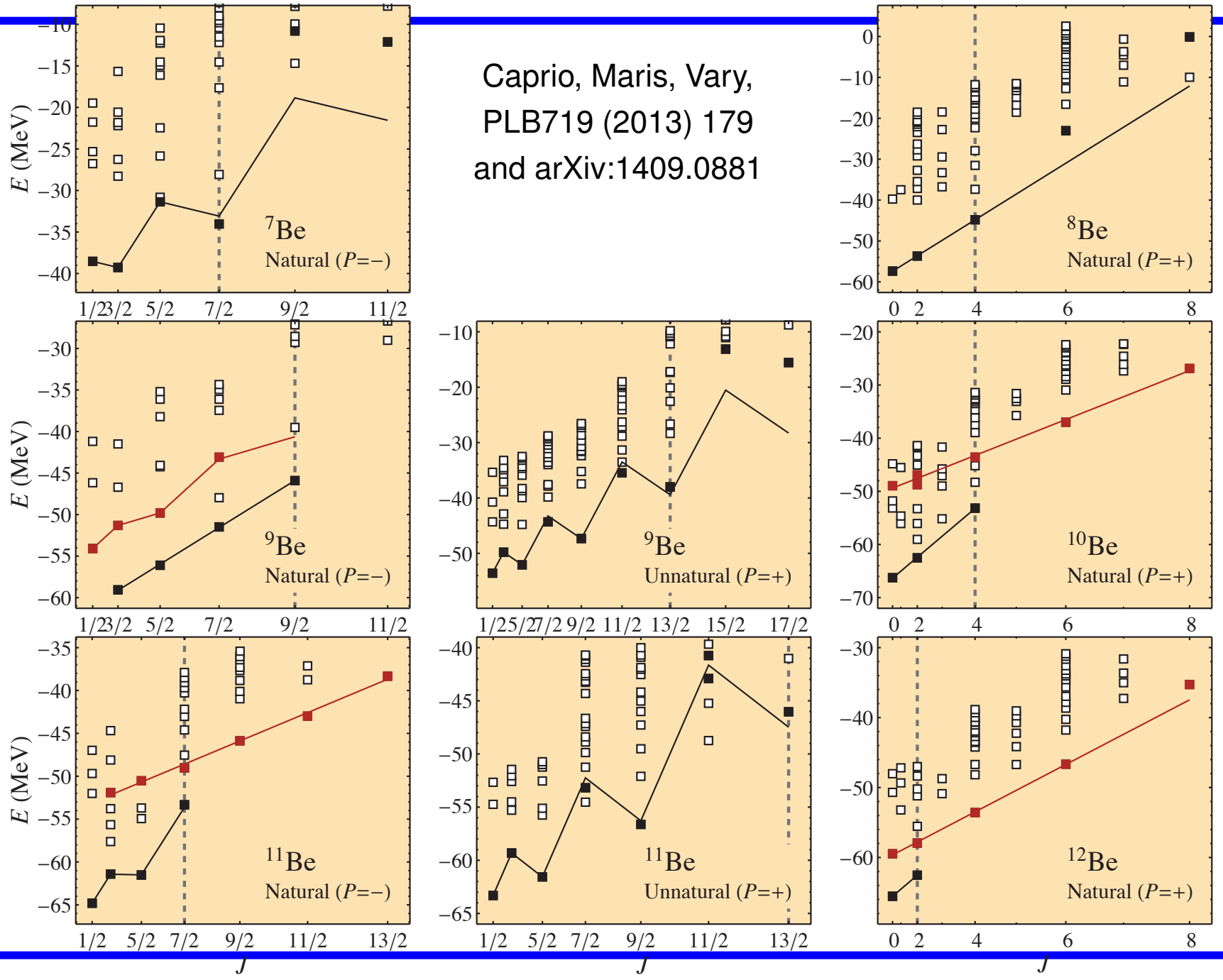
$$\mathcal{Q}(J) = \frac{\frac{3}{4} - J(J+1)}{(J+1)(2J+3)}\,\mathcal{Q}_0$$

$$B(E2; i \to f) = \frac{5}{16\pi}\left\langle J_i, \frac{1}{2}; 2, 0 \middle| J_f, \frac{1}{2}\right\rangle^2 \mathcal{Q}_0^2$$

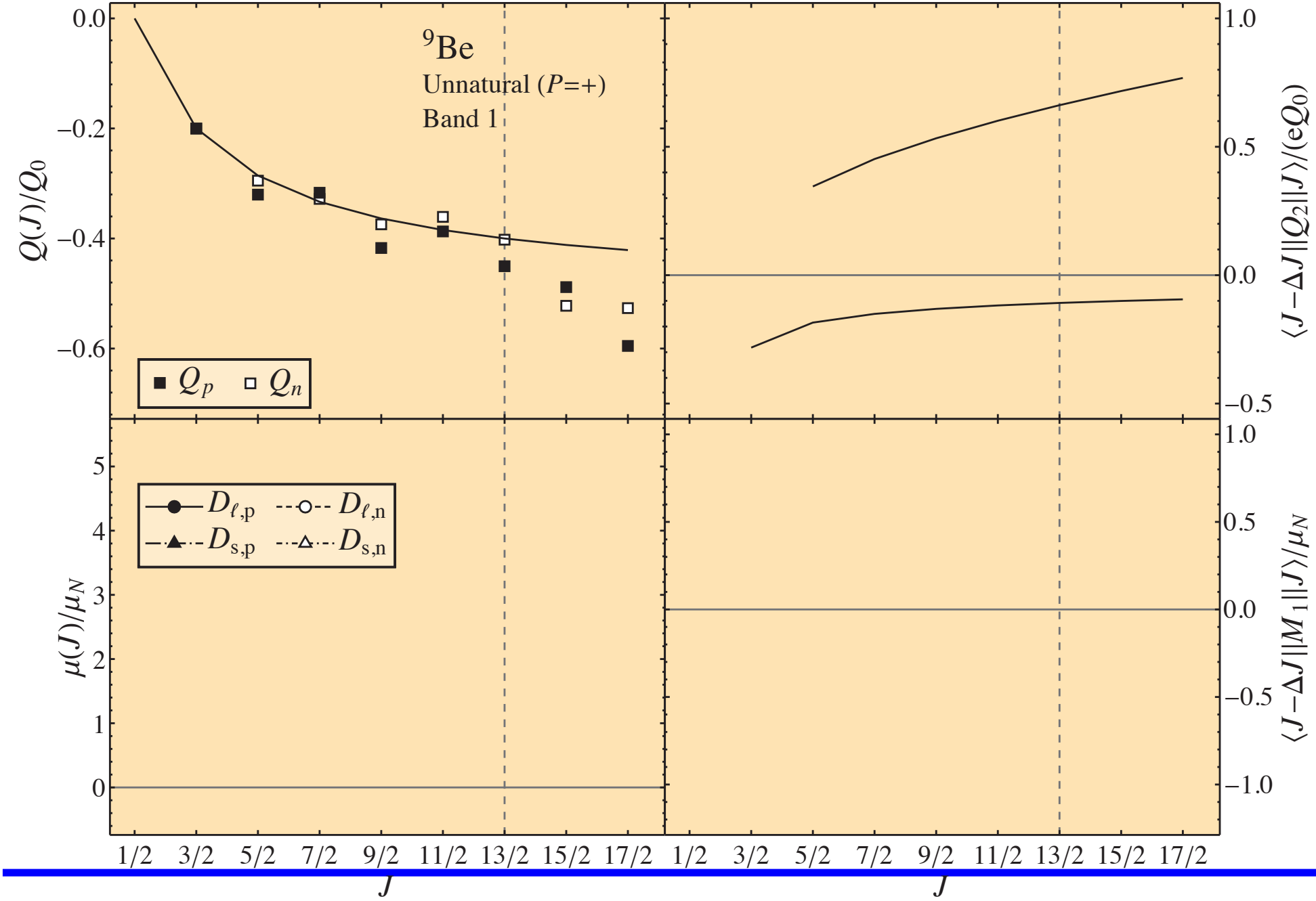
Candidate rotational bands: ^{7}Be–^{12}Be



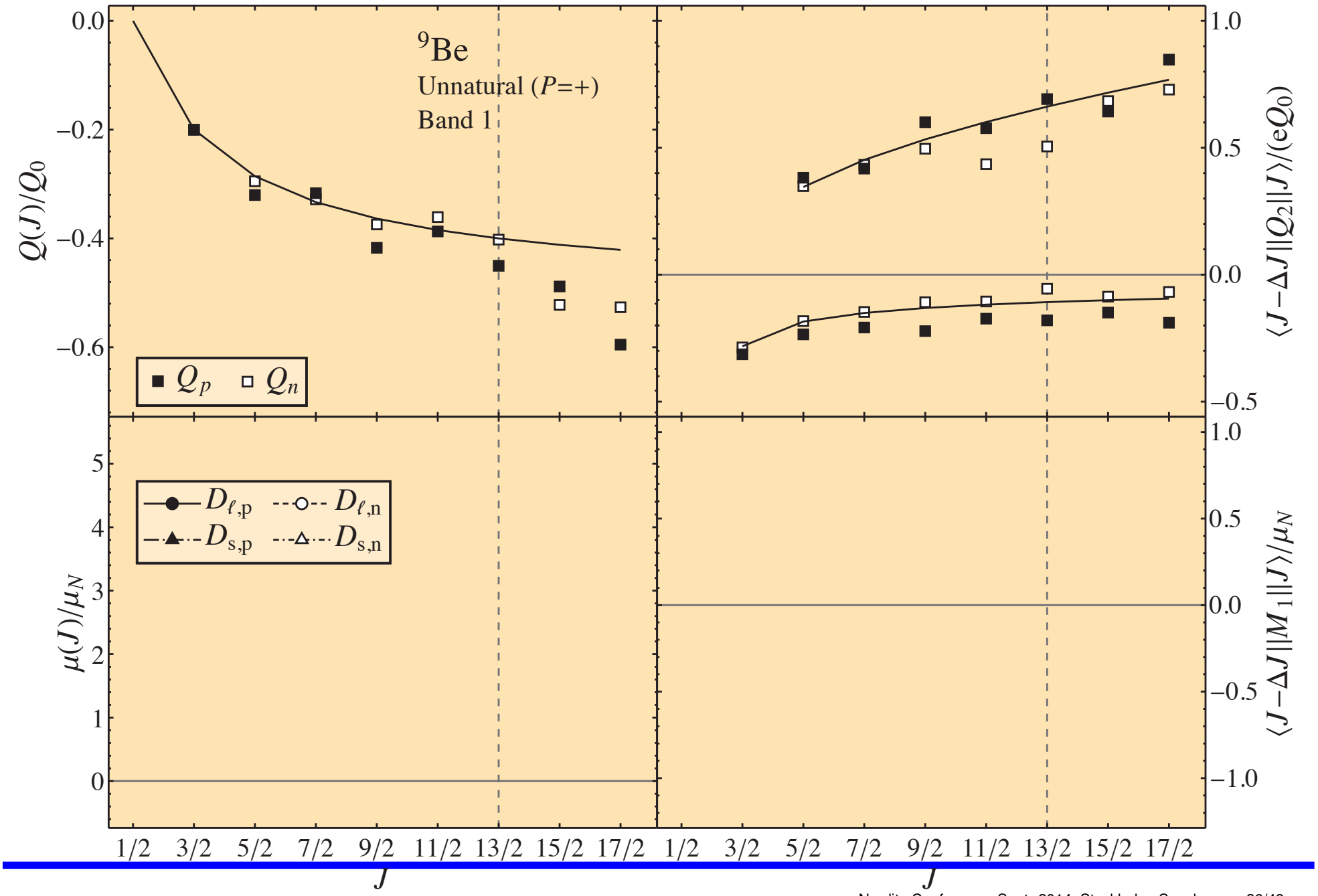
Candidate rotational bands: ^{7}Be–^{12}Be



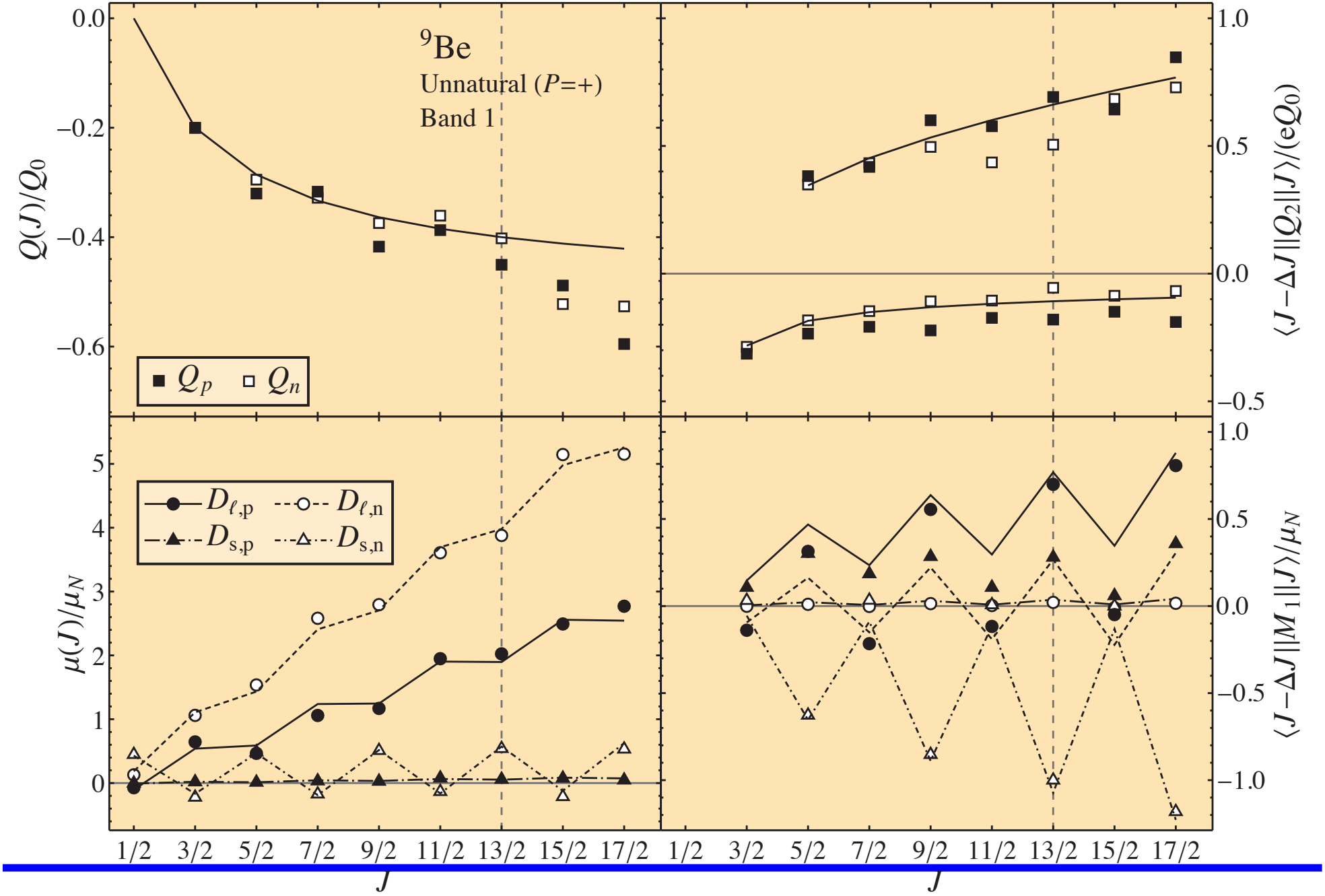
Electromagnetic moments and transitions



Electromagnetic moments and transitions



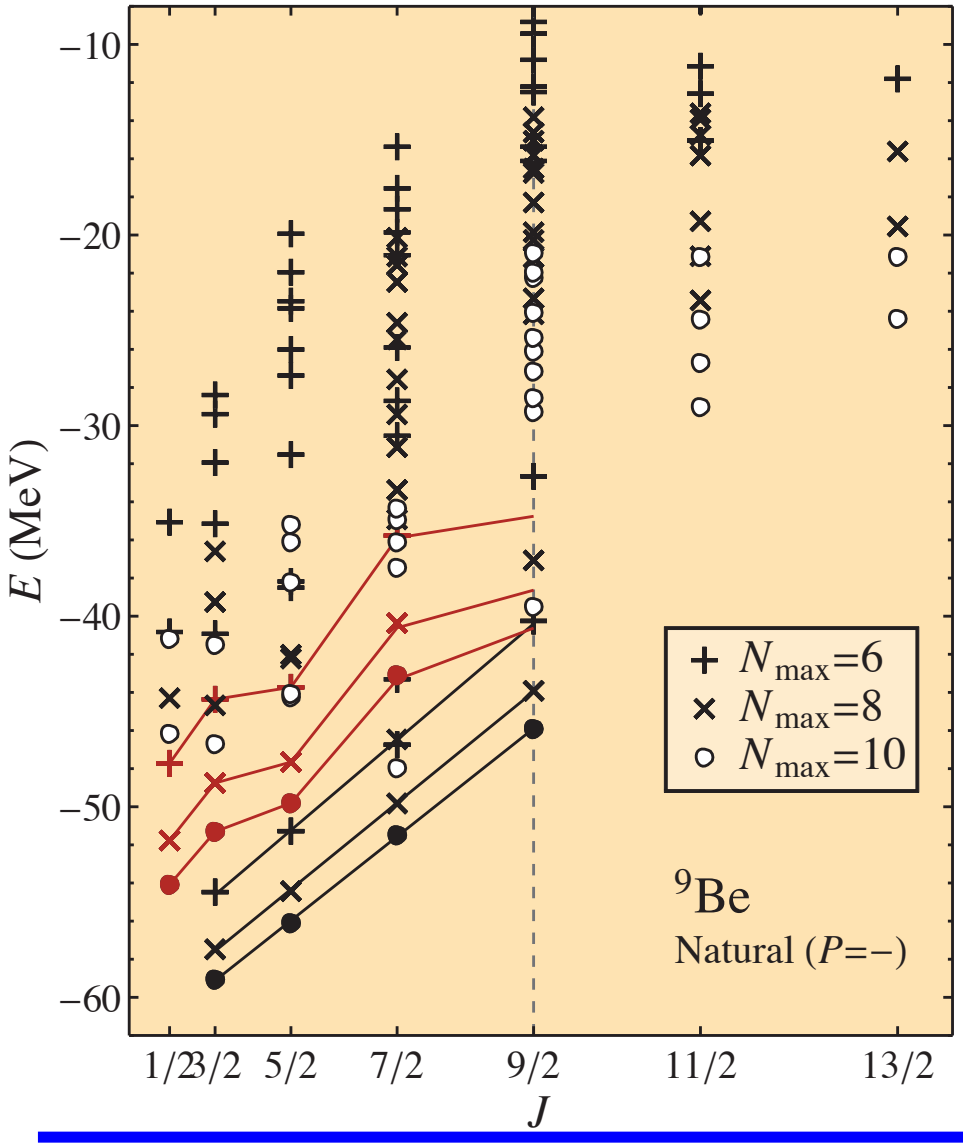
Electromagnetic moments and transitions

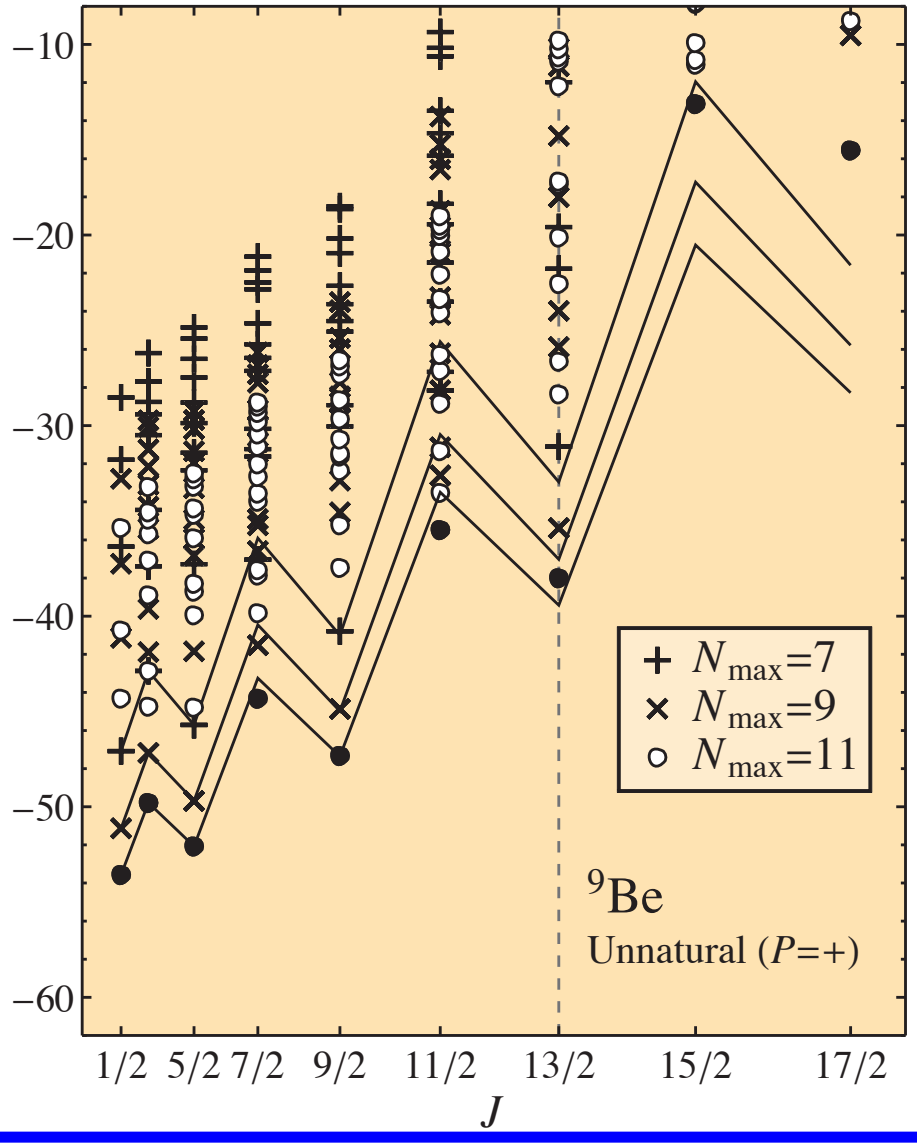


Convergence with basis size? ^{9}Be

Absolute binding energy? NO!

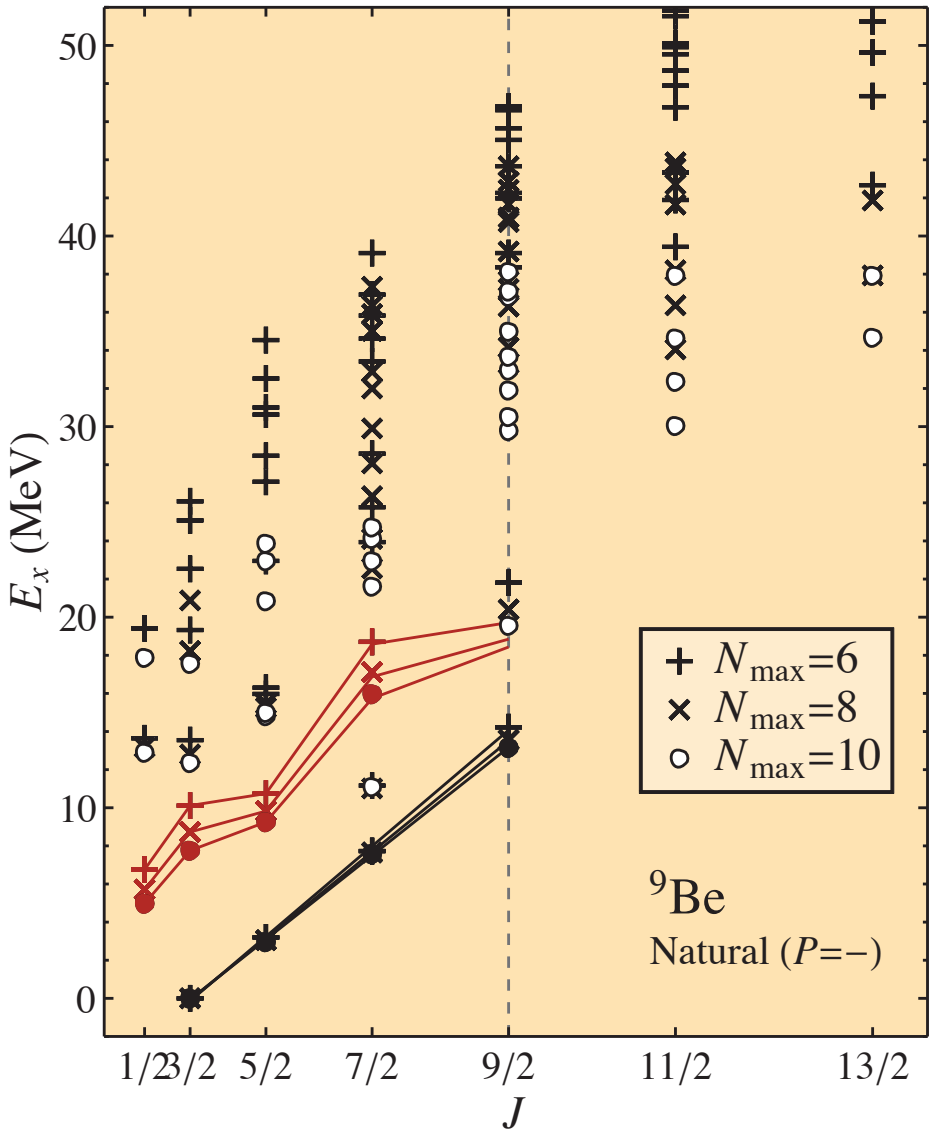
Maris, Caprio, Vary, arXiv:1409.0881

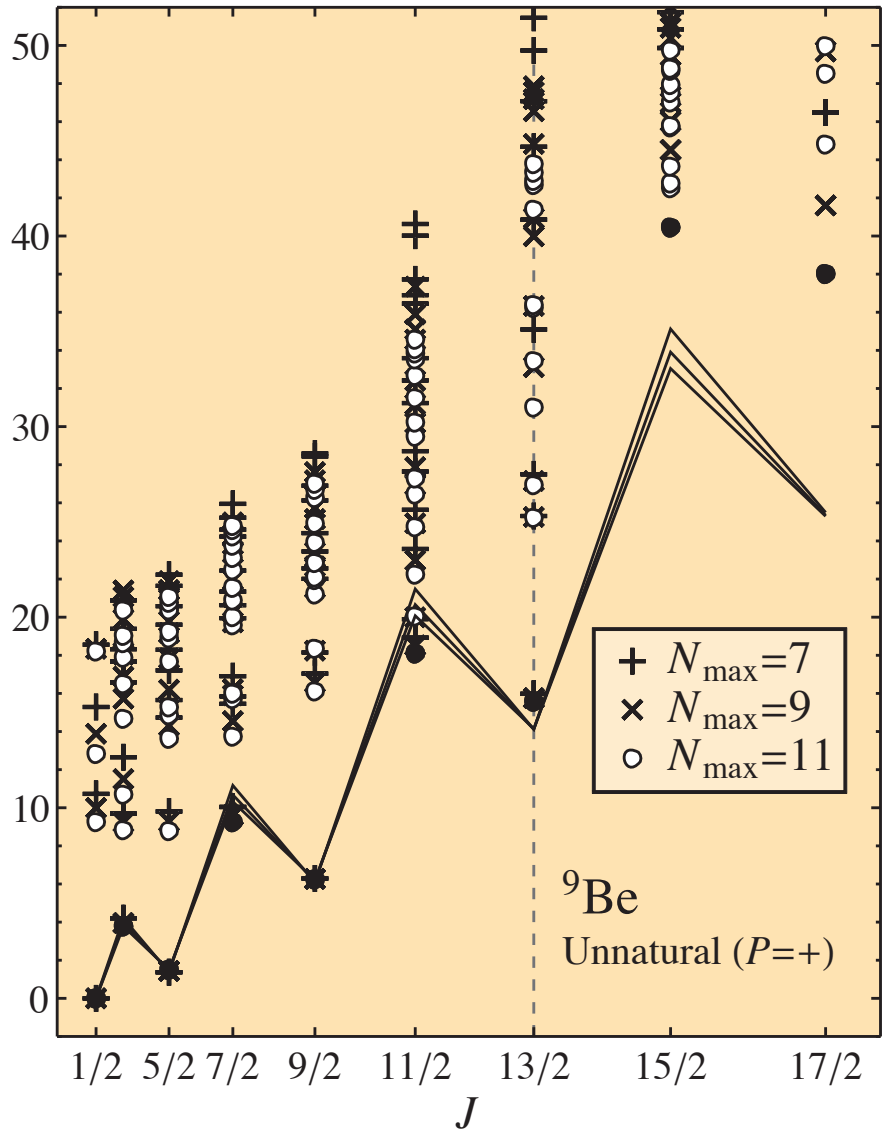




Convergence with basis size? ^{9}Be

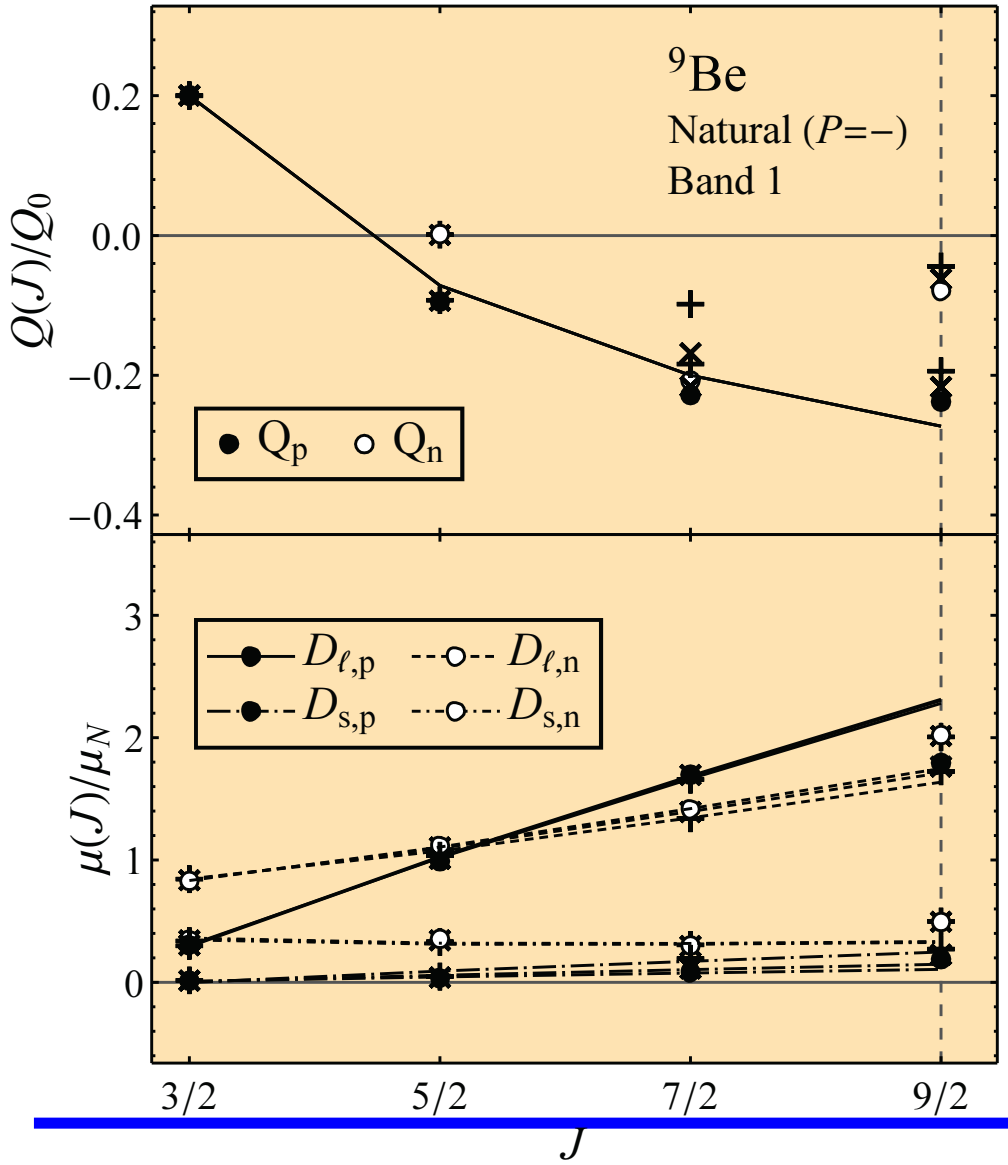
Absolute binding energy? NO! Excitation within band? ~YES

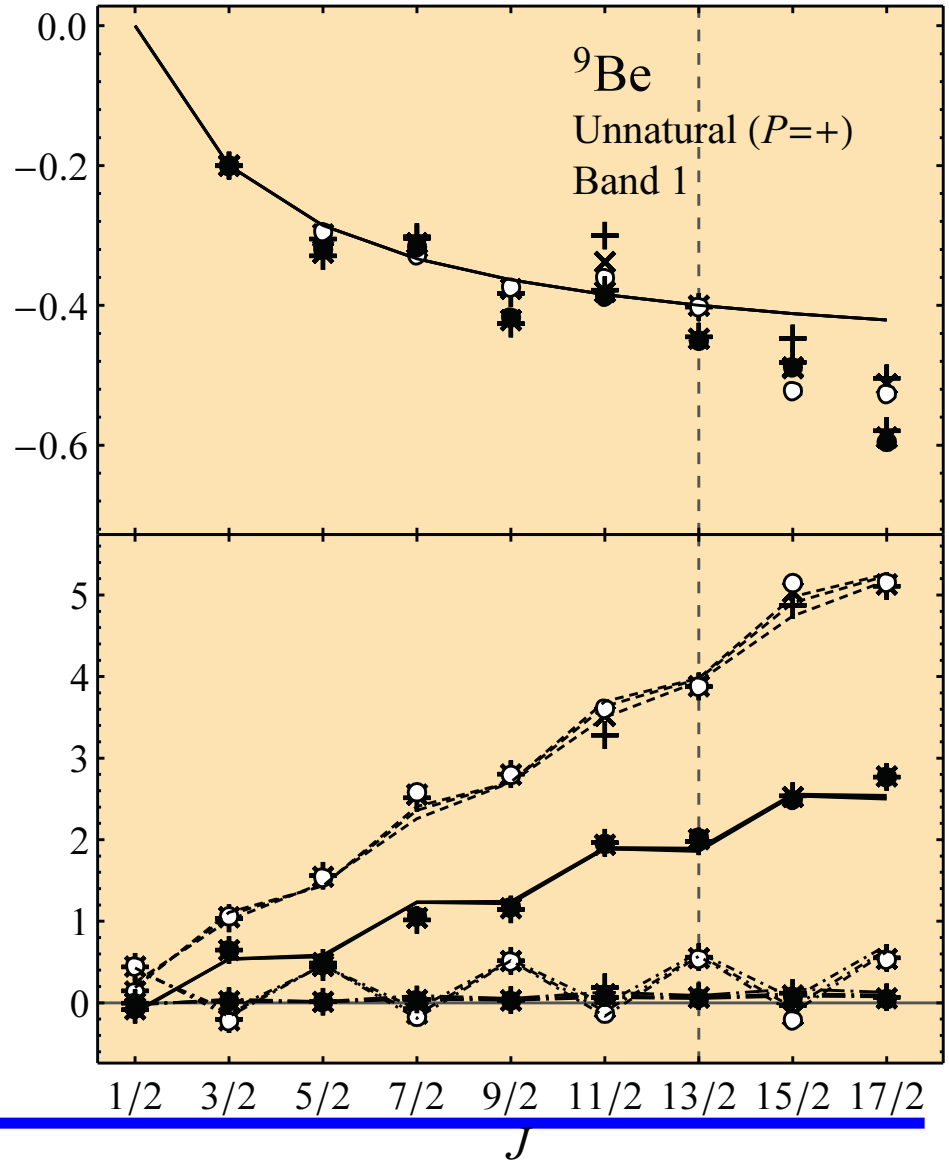




Convergence with basis size? ^{9}Be

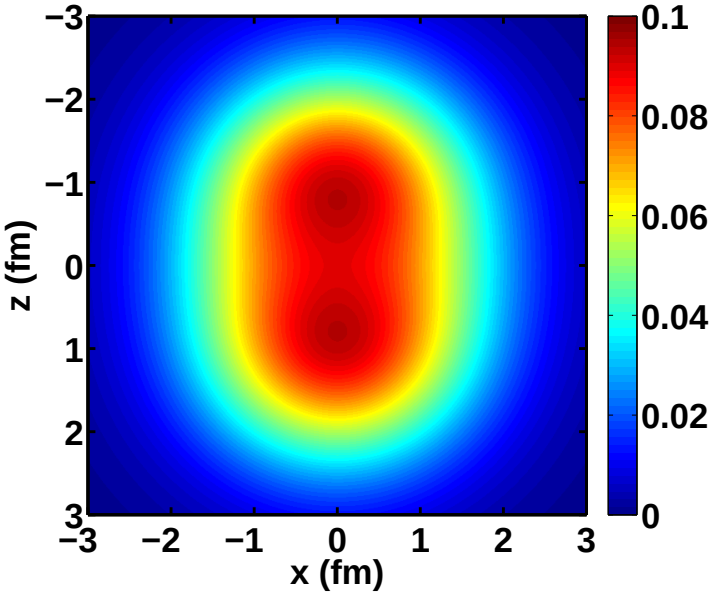
Absolute $E2$? NO! Ratio of $E2$? ~YES Absolute $M1$? ~YES



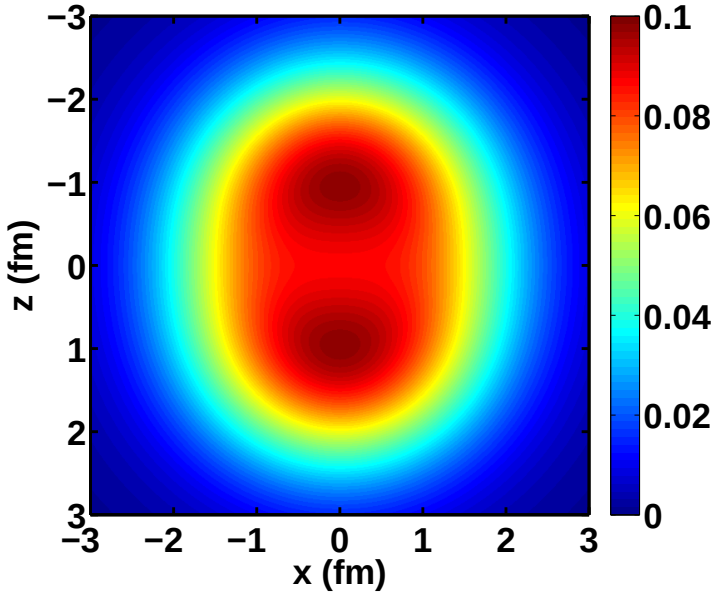


One-body density of 9Be ground state $\left(\frac{3}{2}^-, \frac{1}{2}\right)$

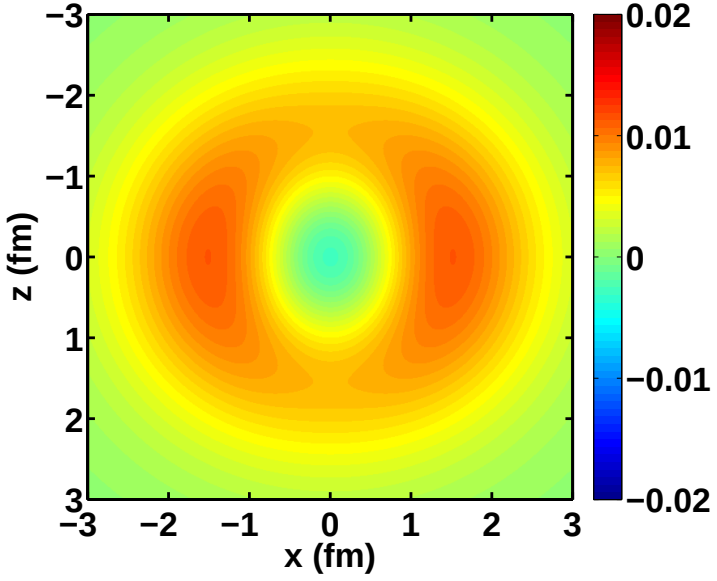
proton



neutron



and their difference



Translationally-invariant proton and neutron densities

Cockrell, PhD thesis, 2012

- Emergence of α clustering
  - extra neutron appears to be in π orbital

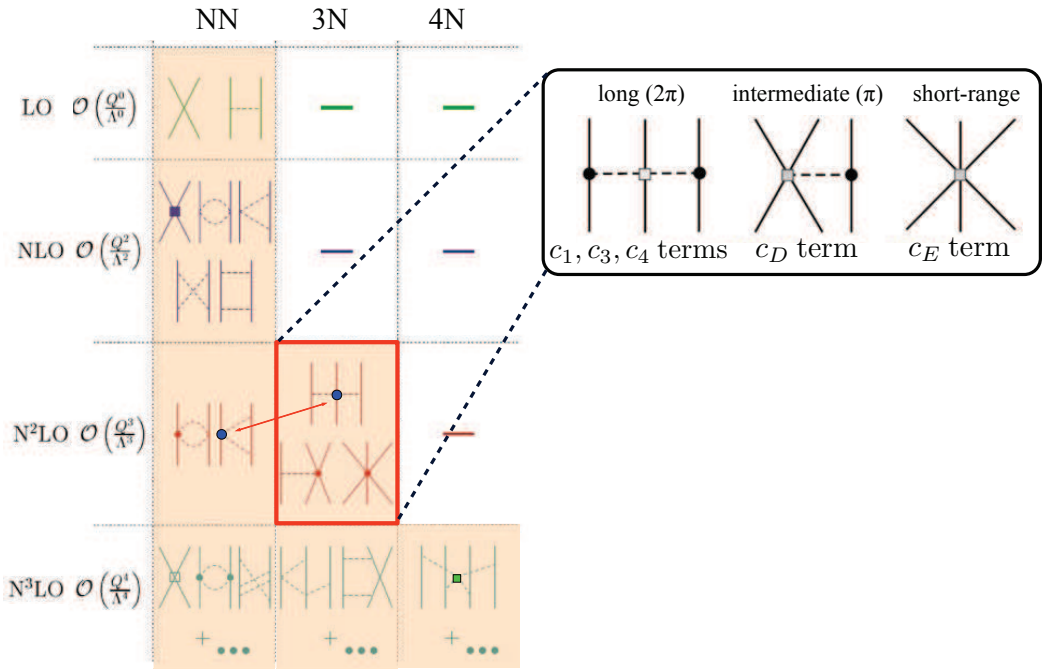
Nuclear interaction from chiral perturbation theory

- Strong interaction in principle calculable from QCD
- Use chiral perturbation theory to obtain effective A-body interaction from QCD Entem and Machleidt, PRC68, 041001 (2003)
  - controlled power series expansion in Q/Λ_χ with $\Lambda_\chi \sim 1$ GeV
  - natural hierarchy for many-body forces

$$V_{NN} \gg V_{NNN} \gg V_{NNNN}$$

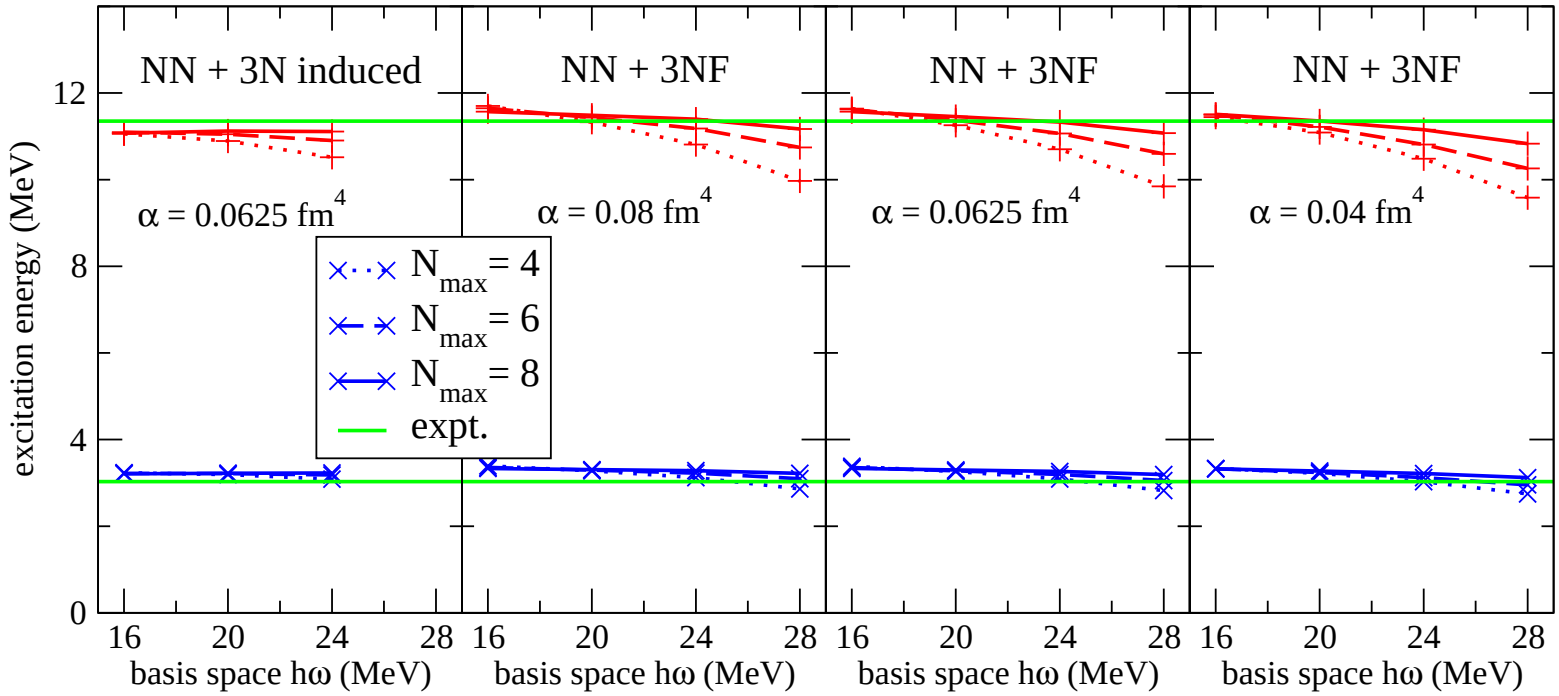
  - in principle no free parameters
    - in practice a few undetermined parameters
  - renormalization necessary

Leading-order 3N forces in chiral EFT



Effect of 3-body forces on rotational excited states ^{8}Be

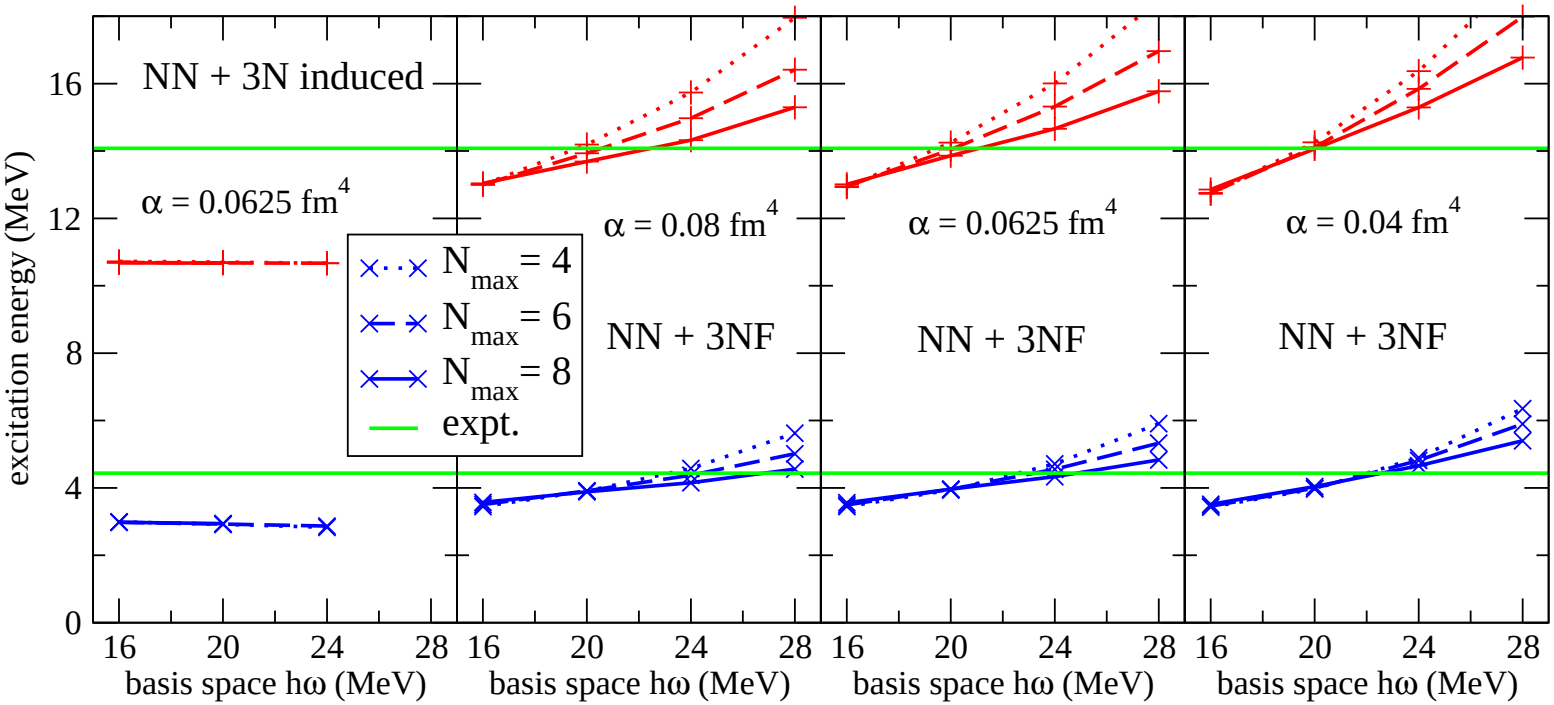
Maris, Aktulga, Binder, Calci, Catalyurek, Langhammer, Ng, Saule, Roth, Vary, Yang
J. Phys. Conf. Ser. 454, 012063 (2013)



- Qualitative agreement with data
- Not converged with explicit 3NF, despite weak $N_{\max}$ dependence
- Ratio's of excitation energies, quadrupole moments and B(E2)'s in agreement with rotational model

Effect of 3-body forces on rotational excited states ^{12}C

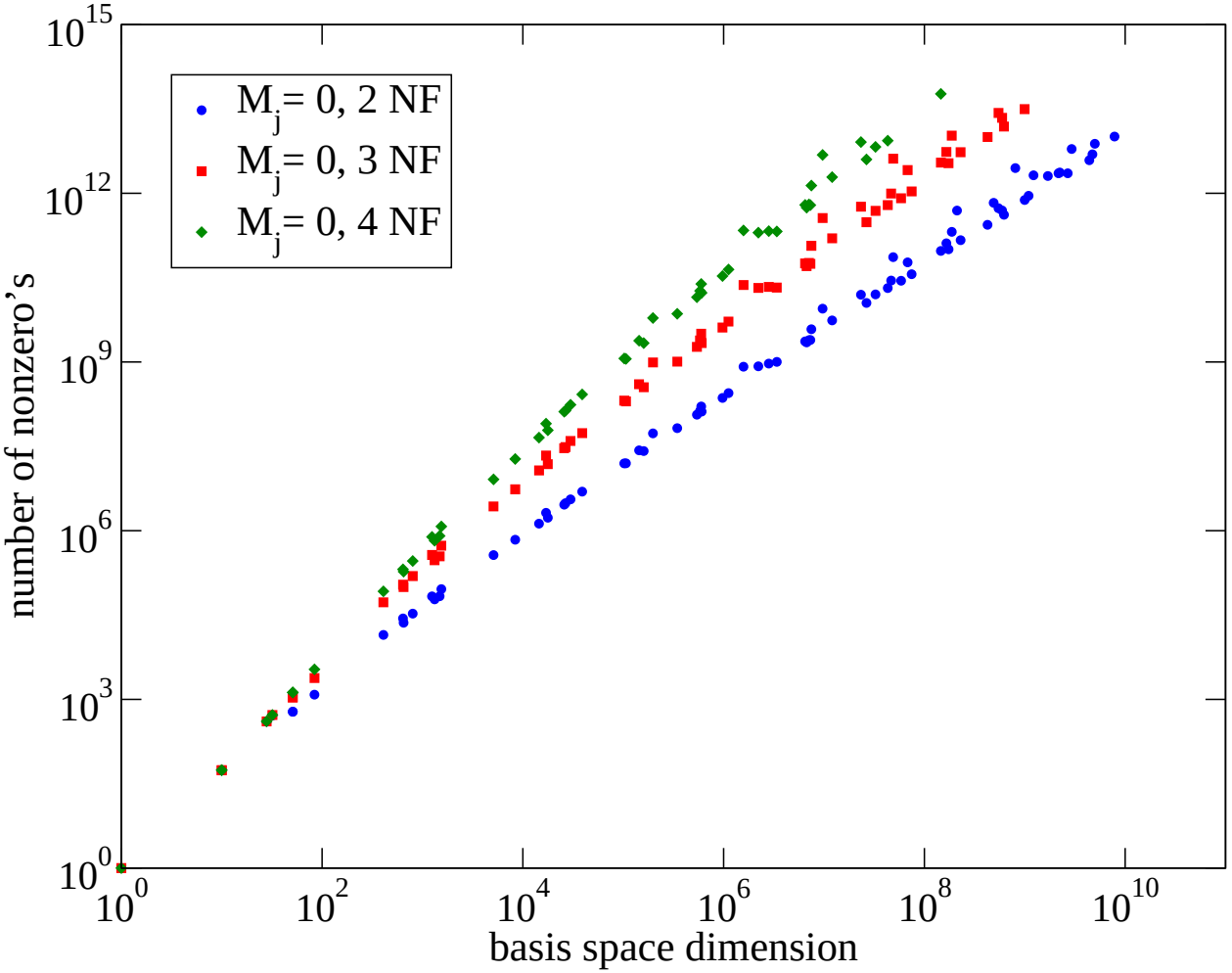
Maris, Aktulga, Binder, Calci, Catalyurek, Langhammer, Ng, Saule, Roth, Vary, Yang
J. Phys. Conf. Ser. 454, 012063 (2013)



- Chiral 3NF improves agreement with data
- Not converged with explicit 3NF, despite weak $N_{\max}$ dependence
- Increase in excitation energy of $(2^+, 0)$ and $(4^+, 0)$ rotational states likely due to increased binding of $(0^+, 0)$

Looking forward: Taming the scale explosion

- Reaching the limit of M-scheme $N_{\max}$ truncation
  - extremely large, extremely sparse matrices

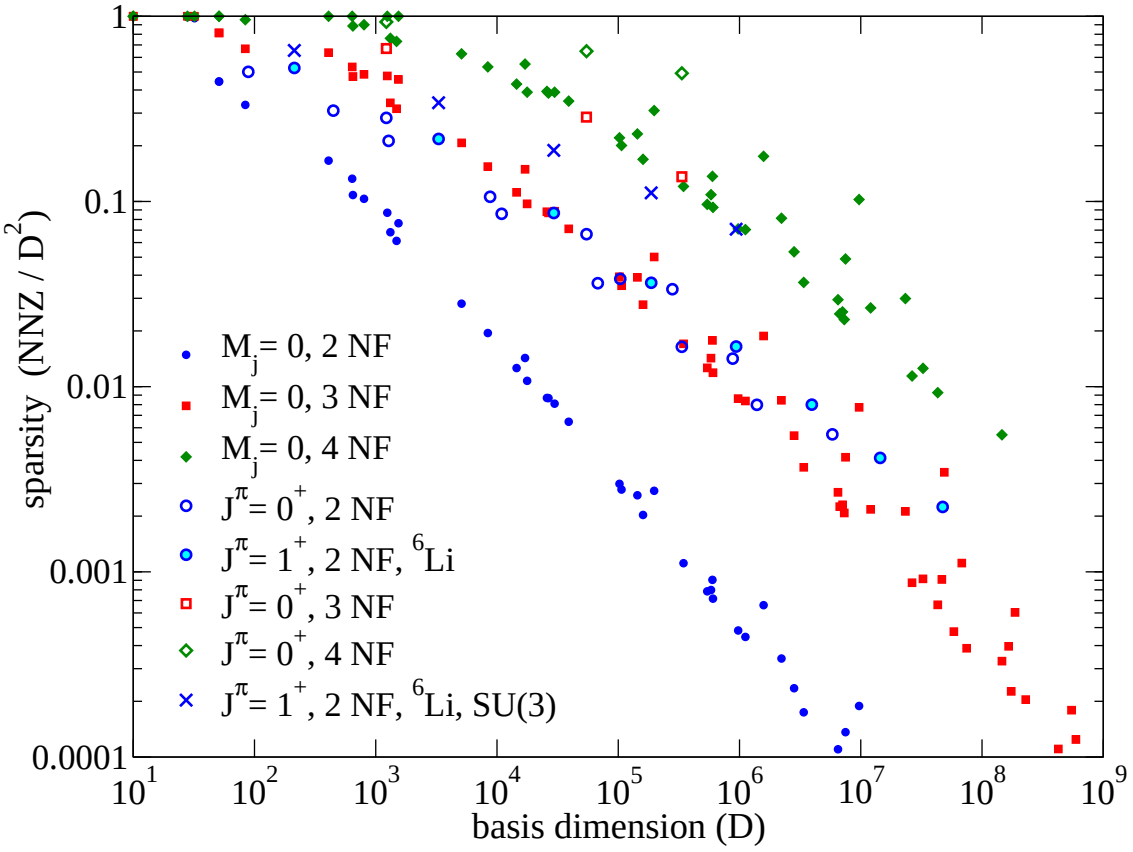


number of nonzero's in M-scheme, $M_j = 0$ for $N = Z$ nuclei from ^{6}Li to ^{20}Ne

- Hopper: 212 TB
  $26 \cdot 10^{12}$
- Edison: 333 TB
  $41 \cdot 10^{12}$
- Titan: 600 TB (CPUs)
  $75 \cdot 10^{12}$
- Mira: 768 TB
  $95 \cdot 10^{12}$
- Blue Waters: 1.4 PB
  $170 \cdot 10^{12}$

Looking forward: *Taming the scale explosion*

- Reaching the limit of M-scheme $N_{\max}$ truncation
- Exploit symmetries to reduce basis dimension
  - Coupled-J basis — Aktulga, Yang, Ng, Maris, Vary, HPCS2011
  - SU(3) basis — Dytrych *et al*, PRL111, 252501 (2013)

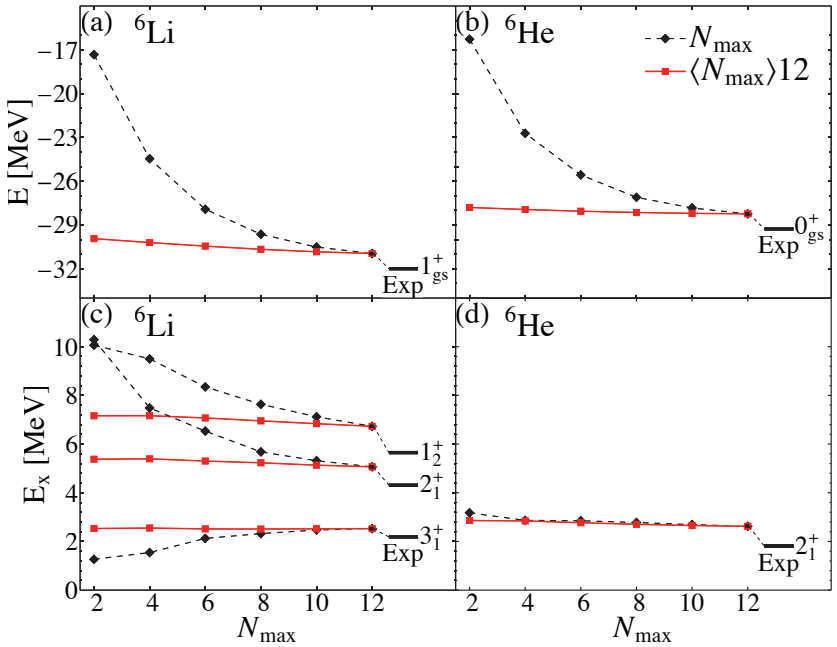


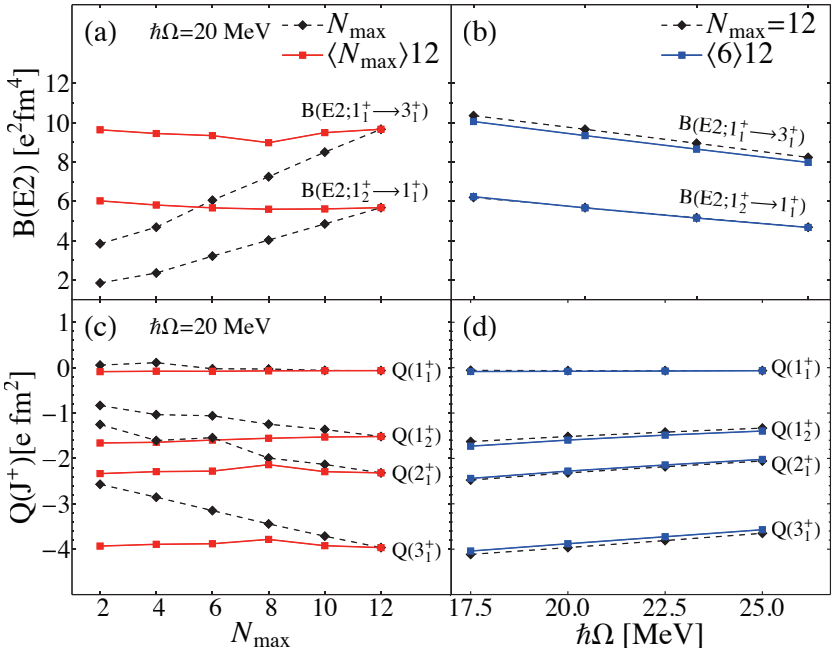
- smaller, but less sparse matrices
- number of nonzero matrix elements often (significantly) larger than in M-scheme
- construction of matrix more costly
- larger memory footprint than in M-scheme

Reducing the basis dimension

- Symmetry-Adapted No-Core Shell Model

Dytrych *et al*, PRL111, 252501 (2013)





- $\langle N_{\max}\rangle 12$ complete basis up to $N_{\max}$, dominant SU(3) irreps up to $N_{\max} = 12$
- Exact factorization (in combination with HO s.p. basis)
- Calculations for ^{12}C and ^{20}Ne in progress

Reducing the basis dimension

- Symmetry-Adapted No-Core Shell Model

  Dytrych *et al*, PRL111, 252501 (2013)

- No-Core Monte-Carlo Shell Model

  Abe, Maris, Otsuka, Shimizu, Utsuno, Vary, PRC86, 054301 (2012)

  - based on FCI truncation, not on $N_{\max}$ truncation
  - reduce basis to (few) hundred highly optimized states
  - coupled-J basis
  - leads to small but dense matrix

- Importance Truncated NCSM Roth, PRC79, 064324 (2009)

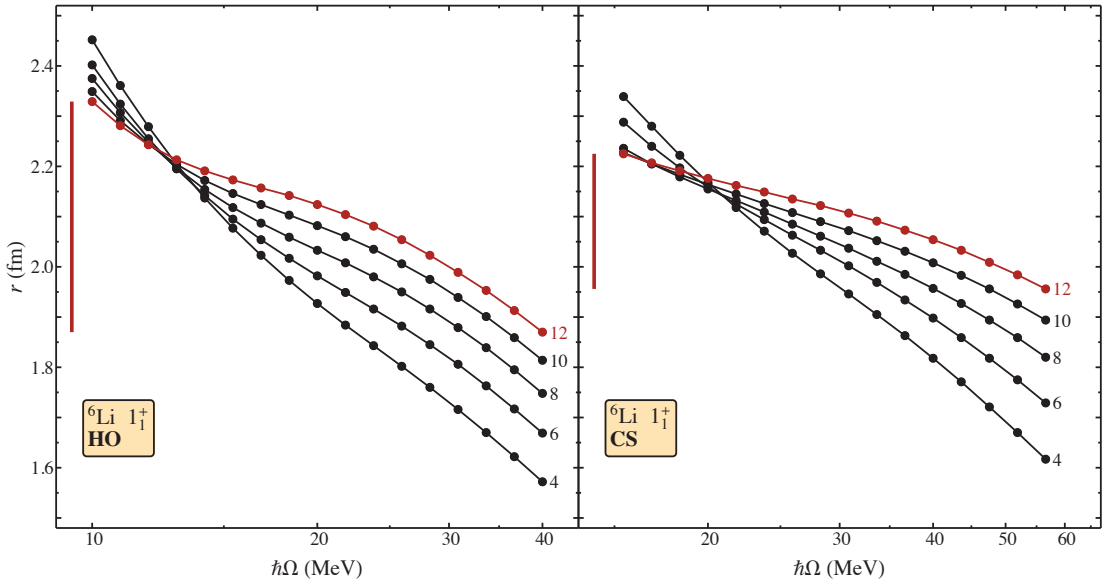
  - based on $N_{\max}$ truncation
  - reduce basis dimension by (several) order(s) of magnitude
  - many-body states single Slater Determinants in M-scheme

Caveat: Uncertainty Quantification

- Can the numerical errors due to reduced basis dimension be quantified within the computation framework?

Beyond Harmonic Oscillator wavefunctions

- Coulomb–Sturmian basis
  - radial basis functions with exponential asymptotic behavior



e.g. Coulomb–Sturmian basis
to improve convergence
of RMS radius,
Caprio, Maris, Vary,
PRC86, 034312 (2012)

- Berggren basis / No-Core Gamow Shell Model
  - incorporate continuum into basis
  - diagonalize complex symmetrix matrix

Conclusions

- No-core Configuration Interaction nuclear structure calculations
  - Binding energy, spectrum, magnetic moments
  - $\langle r^2 \rangle$, $\mathcal{Q}$, transitions, wfns, one-body densities
- Main challenge: construction and diagonalization of extremely large (D $\sim 10^{10}$) sparse (NNZ $\sim 10^{14}$) matrices
- Would not have been possible without collaboration with applied mathematicians and computer scientists
- Emergence of rotational structure
  - Excitation energies (i.e. energy differences)
  - Ratios of quadrupole moments
  - Ratios of quadrupole reduced transition matrix elements
  - Dipole moments $D_{l,p}$, $D_{l,n}$, $D_{s,p}$, and $D_{s,n}$
  - Dipole reduced transition matrix elements
- Convergence of long-range observables remains a challenge